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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jun 03	New e-mail delivery for search results now available
NEWS 4	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 6	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 7	Sep 03	JAPIO has been reloaded and enhanced
NEWS 8	Sep 16	Experimental properties added to the REGISTRY file
NEWS 9	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 10	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11	Oct 24	BEILSTEIN adds new search fields
NEWS 12	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13	Nov 18	DKILIT has been renamed APOLLIT
NEWS 14	Nov 25	More calculated properties added to REGISTRY
NEWS 15	Dec 04	CSA files on STN
NEWS 16	Dec 17	PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17	Dec 17	TOXCENTER enhanced with additional content
NEWS 18	Dec 17	Adis Clinical Trials Insight now available on STN
NEWS 19	Jan 29	Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC
NEWS 20	Feb 13	CANCERLIT is no longer being updated
NEWS 21	Feb 24	METADEX enhancements
NEWS 22	Feb 24	PCTGEN now available on STN
NEWS 23	Feb 24	TEMA now available on STN
NEWS 24	Feb 26	NTIS now allows simultaneous left and right truncation
NEWS 25	Feb 26	PCTFULL now contains images
NEWS 26	Mar 04	SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27	Mar 20	EVENTLINE will be removed from STN
NEWS 28	Mar 24	PATDPAFULL now available on STN
NEWS 29	Mar 24	Additional information for trade-named substances without structures available in REGISTRY
NEWS 30	Apr 11	Display formats in DGENE enhanced
NEWS 31	Apr 14	MEDLINE Reload
NEWS 32	Apr 17	Polymer searching in REGISTRY enhanced
NEWS 33	Apr 21	Indexing from 1947 to 1956 being added to records in CA/CAPLUS
NEWS 34	Apr 21	New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX
NEWS 35	Apr 28	RDISCLOSURE now available on STN
NEWS 36	May 05	Pharmacokinetic information and systematic chemical names added to PHAR
NEWS 37	May 15	MEDLINE file segment of TOXCENTER reloaded
NEWS 38	May 15	Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39	May 16	CHEMREACT will be removed from STN

```
 NEWS 40  May 19  Simultaneous left and right truncation added to WSCA
 NEWS 41  May 19  RAPRA enhanced with new search field, simultaneous left and
                  right truncation

 NEWS EXPRESS  April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:23:59 ON 03 JUN 2003

=> fil reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

FILE 'REGISTRY' ENTERED AT 09:24:08 ON 03 JUN 2003
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    1 JUN 2003  HIGHEST RN 523977-56-2
DICTIONARY FILE UPDATES:   1 JUN 2003  HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09678595.str

L1      STRUCTURE UPLOADED

=> d l1
```
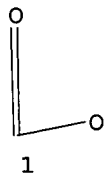
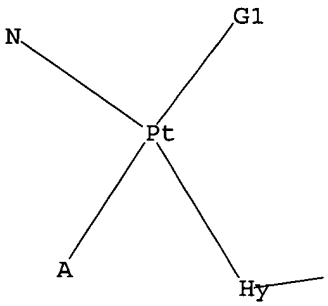

L1 HAS NO ANSWERS
L1 STR





G1 OH,X,[@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:24:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2933 TO ITERATE

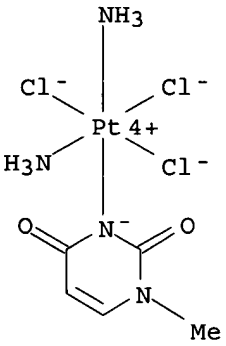
34.1% PROCESSED 1000 ITERATIONS 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 55413 TO 61907
PROJECTED ANSWERS: 29 TO 439

L2 4 SEA SSS SAM L1

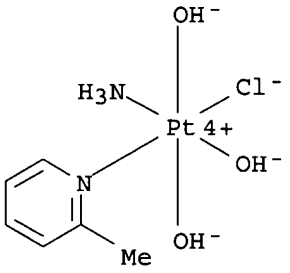
=> d scan

L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum, diamminetrichloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-31)- (9CI)
MF C5 H11 Cl3 N4 O2 Pt
CI CCS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum, amminechlorotrihydroxy(2-methylpyridine)-, (OC-6-34)- (9CI)
MF C6 H13 Cl N2 O3 Pt
CI CCS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

```
=> s l1 ful
FULL SEARCH INITIATED 09:27:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  59422 TO ITERATE

100.0% PROCESSED   59422 ITERATIONS                          272 ANSWERS
SEARCH TIME: 00.00.01

L3          272 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 150.55     150.76

FILE 'CAPLUS' ENTERED AT 09:28:08 ON 03 JUN 2003
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FILE COVERS 1907 - 3 Jun 2003  VOL 138 ISS 23
FILE LAST UPDATED: 2 Jun 2003  (20030602/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l3
L4          169 L3

=> d abs ibib hitstr 1-15
```
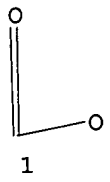
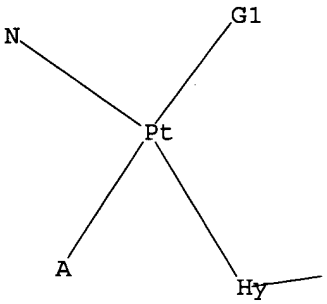





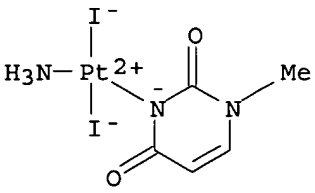
G1 OH,X,[@1]

Structure attributes must be viewed using STN Express query preparation.

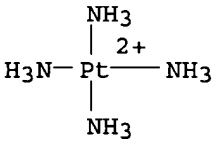
```
=> d his

     (FILE 'HOME' ENTERED AT 09:23:59 ON 03 JUN 2003)

     FILE 'REGISTRY' ENTERED AT 09:24:08 ON 03 JUN 2003
L1             STRUCTURE UPLOADED
L2               4 S L1
L3             272 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 09:28:08 ON 03 JUN 2003
L4             169 S L3

     FILE 'STNGUIDE' ENTERED AT 09:34:44 ON 03 JUN 2003

     FILE 'REGISTRY' ENTERED AT 09:39:54 ON 03 JUN 2003
L5             STRUCTURE UPLOADED

=> s l5 ful sub=l3
FULL SUBSET SEARCH INITIATED 09:40:35 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -    272 TO ITERATE

100.0% PROCESSED     272 ITERATIONS                          143 ANSWERS
SEARCH TIME: 00.00.01

L6             143 SEA SUB=L3 SSS FUL L5

=> d scan
```

L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum(2+), tetraammine-, (SP-4-1)-, bis[(SP-4-1)-amminediiodo(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)platinate(1-)] (9CI)
MF C5 H8 I2 N3 O2 Pt . 1/2 H12 N4 Pt

CM 1

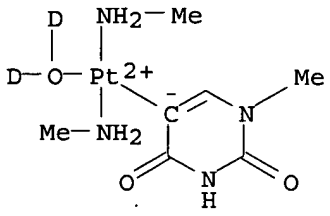


CM 2

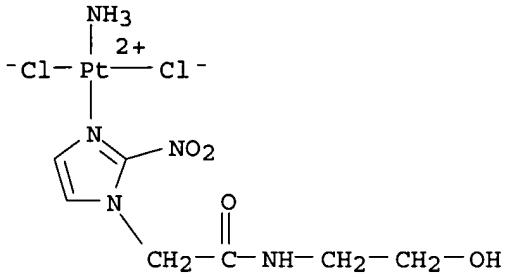


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum(1+), aqua-d2-bis(methanamine)(1,2,3,4-tetrahydro-1-methyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)- (9CI)
MF C7 H15 D2 N4 O3 Pt
CI CCS

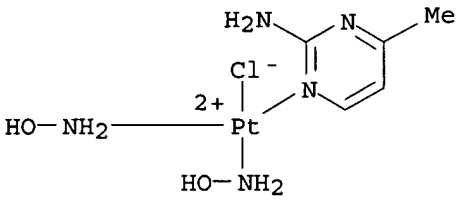


L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum, amminedichloro[N-(2-hydroxyethyl)-2-nitro-1H-imidazole-1-acetamide-N3]-, (SP-4-3)- (9CI)
MF C7 H13 Cl2 N5 O4 Pt
CI CCS



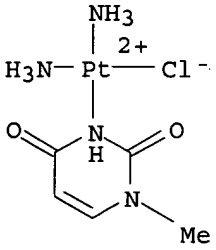
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum(1+), chlorobis(hydroxylamine-N)(4-methyl-2-pyrimidinamine-N1)-, chloride, (SP-4-3)- (9CI)
MF C5 H13 Cl N5 O2 Pt . Cl
CI CCS



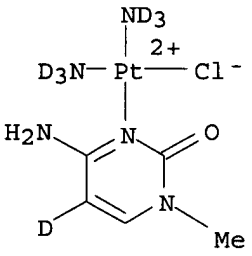
● Cl -

L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum(1+), diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedione-N3)-, (SP-4-3)- (9CI)
MF C5 H12 Cl N4 O2 Pt
CI CCS

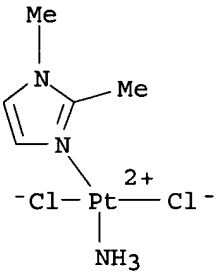


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum(1+), [(4-amino-1-methyl-2(1H)-pyrimidinone-5-d)-N3]di(ammine-d3)chloro-, (SP-4-3)- (9CI)
MF C5 H6 Cl D7 N5 O Pt
CI CCS, COM



L6 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Platinum, amminedichloro(1,2-dimethyl-1H-imidazole-.kappa.N3)-, (SP-4-3)-
(9CI)
MF C5 H11 Cl2 N3 Pt
CI CCS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

```
=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      36.10     396.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00     -29.30

FILE 'CAPLUS' ENTERED AT 09:41:42 ON 03 JUN 2003
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FILE COVERS 1907 - 3 Jun 2003  VOL 138 ISS 23
FILE LAST UPDATED: 2 Jun 2003  (20030602/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> d his

     (FILE 'HOME' ENTERED AT 09:23:59 ON 03 JUN 2003)

     FILE 'REGISTRY' ENTERED AT 09:24:08 ON 03 JUN 2003
L1             STRUCTURE UPLOADED
L2               4 S L1
L3             272 S L1 FUL

     FILE 'CAPLUS' ENTERED AT 09:28:08 ON 03 JUN 2003
L4             169 S L3

     FILE 'STNGUIDE' ENTERED AT 09:34:44 ON 03 JUN 2003

     FILE 'REGISTRY' ENTERED AT 09:39:54 ON 03 JUN 2003
L5             STRUCTURE UPLOADED
L6             143 S L5 FUL  SUB=L3

     FILE 'CAPLUS' ENTERED AT 09:41:42 ON 03 JUN 2003

=> s l6
L7              87 L6

=> d abs ibib hitstr 1-
YOU HAVE REQUESTED DATA FROM 87 ANSWERS - CONTINUE? Y/(N):y
```

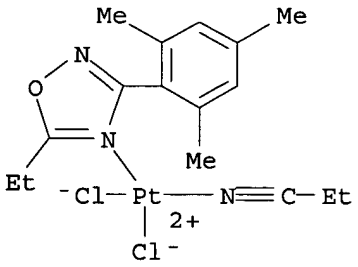
L7 ANSWER 1 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A significant activation of the C.tplbond.N group in organonitriles upon their coordination to a Pt(IV) center was found in the reaction of [PtCl4(RCN)2] (R = Me, Et, CH2Ph) with the nitrile oxides 2,4,6-R'3C6H2CNO (R' = Me, OMe) to give the (1,2,4-oxadiazole)platinum(IV) complexes [PtCl4{cyclic-N:C(R)ON:CC6H2R'3}] (R = Me, R' = Me (1); R = Et, R' = Me (2); R = Et, R' = OMe (3); R = CH2Ph, R' = Me (4)); the [2 + 3] cycloaddn. was performed under mild conditions (unless poor soly. of [PtCl4(RCN)2] precludes the reaction) starting even from complexed MeCN and propionitrile, which exhibit low reactivity in the free state. The reaction between complexes 2-4 and 1 equiv of Ph3P:CHCO2Me in CH2Cl2 leads to the appropriate Pt(II) complexes [PtCl2{cyclic-N:C(R)ON:CC6H2R'3}] (5-7); the redn. failed only in the case of 1 insofar as this complex is insol. in the most common org. solvents. All the Pt compds. were characterized by elemental analyses, FAB mass spectrometry, and IR and 1H, 13C{1H}, and 195Pt NMR spectroscopies, and three of them also by x-ray crystallog. The oxadiazoles formed in the metal-mediated reaction were liberated almost quant. from their Pt(IV) complexes by reaction of the latter (complexes 2-4) with an excess of pyridine in CHCl3, giving free 1,2,4-oxadiazoles and trans-[PtCl4(pyridine)2]. The sequence of the Pt(IV)-mediated [2 + 3] cycloaddn. and the liberation opens up an alternative route for the prepn. of this important class of heterocycles.

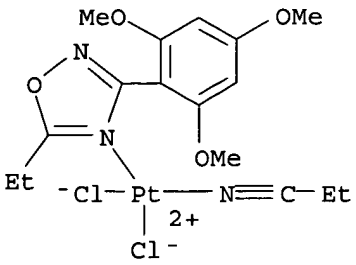
ACCESSION NUMBER: 2003:29980 CAPLUS
DOCUMENT NUMBER: 138:230968
TITLE: A Route to 1,2,4-Oxadiazoles and Their Complexes via Platinum-Mediated 1,3-Dipolar Cycloaddition of Nitrile Oxides to Organonitriles
AUTHOR(S): Bokach, Nadezhda A.; Khripoun, Anatolii V.; Kukushkin, Vadim Yu.; Haukka, Matti; Pombeiro, Armando J. L.
CORPORATE SOURCE: Centro de Quimica Estrutural, St. Petersburg State University, Lisbon, 1049-001, Port.
SOURCE: Inorganic Chemistry (2003), 42(3), 896-903
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **500994-80-9 500994-81-0**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (formation in attempted cycloaddn. of (nitrile)platinum(II) complex with nitrile oxide)

RN 500994-80-9 CAPLUS
CN Platinum, dichloro[5-ethyl-3-(2,4,6-trimethylphenyl)-1,2,4-oxadiazole-.kappa.N4](propanenitrile)-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 500994-81-0 CAPLUS
CN Platinum, dichloro[5-ethyl-3-(2,4,6-trimethoxyphenyl)-1,2,4-oxadiazole-.kappa.N4](propanenitrile)-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

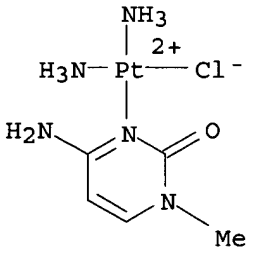
L7 ANSWER 2 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn., the crystal structure detn. of two modifications, and the soln. behavior of the mixed nucleobase complex trans-[Pt(NH3)2(1-MeC-N3)(9-EtGH-N7)](ClO4)2.cntdot.nH2O (n = 1.4 (2a) and 0 (2b)) with 1-MeC = 1-methylcytosine and 9-EtGH = 9-ethylguanine are reported. The compd. is a model for the most abundant interstrand cross-link of trans-Pt(NH3)2Cl2 (Transplatin) with double-stranded DNA. Characteristic features of this compd. are the near-coplanarity of the two nucleobases and the intracomplex H bond between the exocyclic groups N(4)H2 of 1-MeC and O(6) of 9-EtGH. Geometrical parameters responsible for the length of this H bond were studied. The compd. can be considered a metal-modified Hoogsteen pair of cytosine and guanine. Its potential relevance to platinated DNA triplexes is also briefly discussed.

ACCESSION NUMBER: 2002:857712 CAPLUS
DOCUMENT NUMBER: 138:197737
TITLE: Model of the most abundant DNA interstrand cross-link of Transplatin: X-ray structures of two modifications and H bonding behavior in the solid state and in solution of trans-[Pt(NH3)2(1-MeC-N3)(9-EtGH-N7)](ClO4)2.cntdot.nH2O (1-MeC = 1-methylcytosine; 9-EtGH = 9-ethylguanine)
AUTHOR(S): Erxleben, Andrea; Metzger, Susanne; Britten, James F.; Lock, Colin J. L.; Albinati, Alberto; Lippert, Bernhard
CORPORATE SOURCE: Department of Chemistry, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: Inorganica Chimica Acta (2002), 339, 461-469
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:197737

IT **98920-59-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with ethylguanine)

RN 98920-59-3 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



⊕ Cl -

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

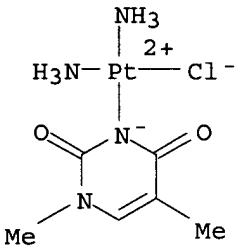
L7 ANSWER 3 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Methylation at the N7 position is one of the most frequently naturally occurring modifications of guanosine. This alteration drastically changes the hydrogen bonding and acid-base properties of the guanine nucleobase. Here we show on the example of the model nucleobase 7,9-dimethylguanine that due to blockage of N7 of the purine ring, new hydrogen bonding patterns occur on the minor groove binding face of this nucleobase involving the ring nitrogen N3 and the exocyclic amino group NH2. The free 7,9-dimethylguaninium ion and several trans-platinum(II) complexes of the this ligand are presented and discussed.

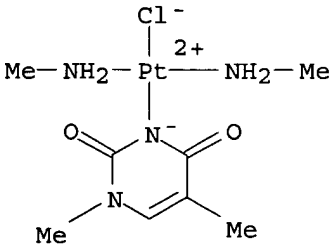
ACCESSION NUMBER: 2002:857700 CAPLUS
DOCUMENT NUMBER: 138:169996
TITLE: Hydrogen bonding patterns of 7,9-dimethylguanine and its transplatinum(II) complexes
AUTHOR(S): Sigel, Roland K. O.; Freisinger, Eva; Abbate, Michele; Lippert, Bernhard
CORPORATE SOURCE: Department of Biochemistry and Molecular Biophysics, Columbia University, New York, NY, 10032-3702, USA
SOURCE: Inorganica Chimica Acta (2002), 339, 355-365
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149951-64-4 150120-54-0 220760-69-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with dimethylguanine; crystal structure and hydrogen bonding patterns of 7,9-dimethylguanine and its trans-platinum(II) complexes)

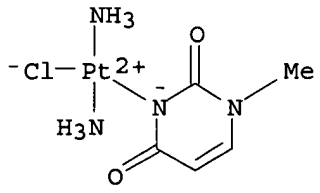
RN 149951-64-4 CAPLUS
CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 150120-54-0 CAPLUS
CN Platinum, chloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)bis(methanamine)-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 220760-69-0 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 87 CAPLUS COPYRIGHT 2003 ACS

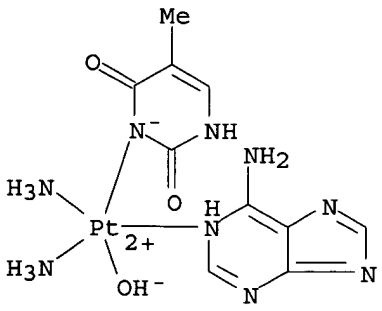
AB Chloroform- and Freon-sol. mixed thymine, adenine complexes trans-[Pt(MeNH2)2(ChmT-N3)(ChmA-N1)]NO3 (2) and trans-[Pt(MeNH2)2(ChmT-N3)(TBDMS-ado-N1)]BF4 (3) (ChmT = anion of 1-cyclohexylmethylthymine ChmTH, ChmA = 9-cyclohexylmethyladenine, TBDMS-ado = 2',3',5'-tri-tert-butyldimethylsilyladenosine) were prepd. and characterized to study their propensity to undergo Hoogsteen and/or reversed Hoogsteen pairing in soln. with free ChmTH and free 3',5'-diacetyl-2'-deoxyuridine, resp. No Hoogsteen or reversed Hoogsteen pairing between 2 and ChmT takes place in CDCl3. In Freon, partial H bonding between N1 platinated TBDMS-ado and 3',5'-diacetyl-2'-deoxyuridine as well as its [3-15N] labeled analog is unambiguously obsd. only <150 K. Comparison of 1J (15N-1H) coupling consts. of 3',5'-diacetyl-2'-deoxyuridine involved in Hoogsteen pairing with free and N1 platinated adenine suggests that the interaction is inherently weaker in the case of platinated adenine. To better understand the complete absence of H bonding between the ChmA ligand in 2 and free ChmTH, ab initio calcns. (gas phase, 0 K) were carried out for Hoogsteen pairs involving adenine (A) and thymine (T), as well as simplified analogs of 2 and T, both in the presence and absence of counteranions. The data strongly suggest that redn. of the effective pos. charge of the heavy metal ion Pt2+ by counterions diminishes interaction energies. With regard to mixts. of 2 and ChmTH in CHCl3, this implies that ion pair formation between the cation of 2 and NO3- may be responsible for the lack of any measurable Hoogsteen pairing in this solvent.

ACCESSION NUMBER: 2002:343911 CAPLUS
DOCUMENT NUMBER: 137:72066
TITLE: Loss of Hoogsteen Pairing Ability upon N1 Adenine Platinum Binding
AUTHOR(S): Schmidt, Kathrin S.; Reedijk, Jan; Weisz, Klaus; Janke, Eline M. Basilio; Sponer, Judit E.; Sponer, Jiri; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, 44221, Germany
SOURCE: Inorganic Chemistry (2002), 41(11), 2855-2863
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:72066

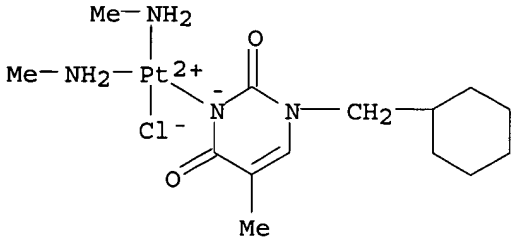
IT **439113-78-7**
RL: PRP (Properties)
(Hoogsteen pairing ability with thymine from calcd. base pairing interaction energy)

RN 439113-78-7 CAPLUS

CN Platinum, diamminehydroxy(5-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)(1H-purin-6-amine-.kappa.N1)-, (SP-5-13)- (9CI) (CA INDEX NAME)



IT **263257-48-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with 9-cyclohexylmethyladenine or tri-tert-butyldimethylsilyladenosine in presence of silver salt)
RN 263257-48-3 CAPLUS
CN Platinum, chloro[1-(cyclohexylmethyl)-5-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3]bis(methanamine)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

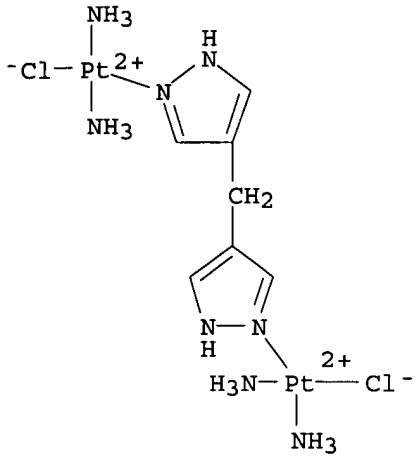
L7 ANSWER 5 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Two cationic multinuclear platinum complexes linked with the 4,4'-dipyrazolylmethane (dpzm) ligand, trans-[{Pt(NH3)2Cl}2-.mu.-dpzm]Cl2 (di-Pt) and trans-[trans-{Pt(NH3)2Cl}2{trans-[Pt(NH3)2(.mu.-dpzm)2]}]Cl4 (tri-Pt), have been synthesized. Both complexes show activity in the murine leukemia cell line L1210 (IC50 = 3.8 and 2.5 .mu.M, resp.) and the cisplatin-resistant subline L1210/DDP (8.8 and 3.6 .mu.M), and in the human ovarian carcinoma 2008 (2.5 and 17.8 .mu.M) and its cisplatin-resistant subline C13*5 (20.9 and 37.7 .mu.M). Both complexes show high levels of uptake into 2008 cells, when administered at 100 .mu.M, but significantly reduced uptake in the cisplatin-resistant cell line C13*5 (di-Pt, 66% decrease; tri-Pt, 42%; cisplatin, 86%). Both complexes form very high levels of DNA interstrand cross-links in vitro, with 50% interstrand crosslinking obsd. at far lower concns. (di-Pt, 12 nM; tri-Pt, 22 nM) than cisplatin (450 nM). It is proposed that the higher extent of interstrand crosslinking may be due to the rigid nature of the dpzm linking ligand, which prevents the complexes from forming short-range intrastrand adducts, like the GpG adduct formed by cisplatin. The results of this study indicate the importance of the flexibility of the linking ligand for the cytotoxicity of di- and trinuclear platinum anti-cancer complexes.

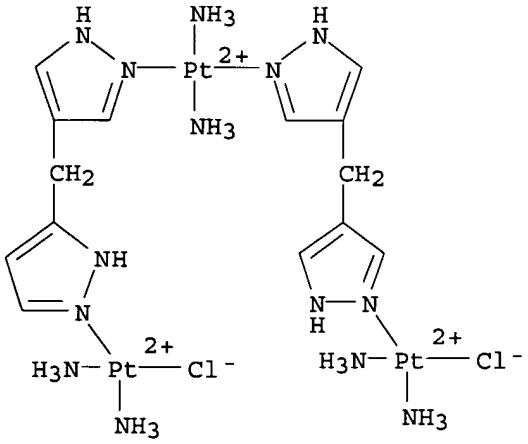
ACCESSION NUMBER: 2002:290106 CAPLUS
DOCUMENT NUMBER: 137:195136
TITLE: Synthesis, cytotoxicity, cell uptake and DNA interstrand cross-linking of 4,4'-dipyrazolylmethane-linked multinuclear platinum anti-cancer complexes
AUTHOR(S): Wheate, Nial J.; Cullinane, Carleen; Webster, Lorraine K.; Collins, J. Grant
CORPORATE SOURCE: School of Chemistry, University College, University of New South Wales, Australian Defence Force Academy, Canberra, 2600, Australia
SOURCE: Anti-Cancer Drug Design (2001), 16(2/3), 91-98
CODEN: ACDDEA; ISSN: 0266-9536
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **453522-73-1P 453522-75-3P**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis, cytotoxicity, cell uptake and DNA interstrand crosslinking of dipyrazolylmethane-linked multinuclear platinum anticancer complexes)

RN 453522-73-1 CAPLUS
CN Platinum, tetraamminedichloro[.mu.-[4,4'-methylenebis[1H-pyrazole-.kappa.N2]]]di-, stereoisomer (9CI) (CA INDEX NAME)



RN 453522-75-3 CAPLUS
CN Platinum, hexaamminedichlorobis[.mu.-[4,4'-methylenebis[1H-pyrazole-.kappa.N2]]tri-, stereoisomer (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 87 CAPLUS COPYRIGHT 2003 ACS
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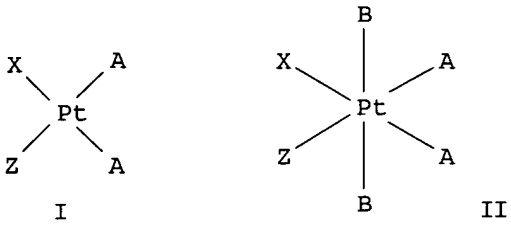


AB The present invention relates to Pt antitumor drugs. In particular, it relates to Pt complexes I or II or a pharmaceutically acceptable salt thereof wherein each A is independently an anion, each B is independently halo, hydroxy, carboxylate, carbamate or a carbonate ester, Z is a substituted 5- or 6-membered, heterocyclic moiety wherein at least one substituent sterically hinders access of the Pt atom to a DNA strand of a tumor cell, and wherein Z is other than pyridine, and X is NH3 or mono- or dialkyl-substituted NH3, which are active against human cancer cells and have improved aq. soly. and activity. Example complexes which are prepd. include cis-[PtII(NH3)Cl2(L)] (L = 3,5-dimethylpyrazole, 1-methylimidazole, 3,5-dimethylisoxazole, 2,3-dimethylpyrazine, etc.) or (OC-6-43)-[PtIV(NH3)Cl2(OH)2(L)] (L = 3,5-dimethylpyrazole, 1-methylimidazole, 2,3-dimethylpyrazine) or (OC-6-43)-[PtIV(NH3)Cl2(OAc)2(L)] (L = 2,3-dimethylpyrazine). The aq. soly. of the complexes at ambient conditions are greater than that of cisplatin. The activity of the complexes in inhibiting human cell lines is comparable to that of prior art compds., at least in some cell lines. Resistance factors with respect to 41M/41MR are particularly favorable for some of the complexes.

ACCESSION NUMBER: 2002:275998 CAPLUS
DOCUMENT NUMBER: 136:288219
TITLE: Platinum ammine complexes or derivatives with improved aqueous solubility and activity as antitumor agents
INVENTOR(S): Wong, Ernest S. Y.; Giandomenico, Christen M.
PATENT ASSIGNEE(S): Anormed Inc., Can.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

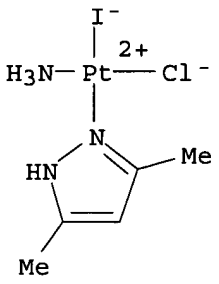
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028871	A1	20020411	WO 2001-US30838	20011002

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

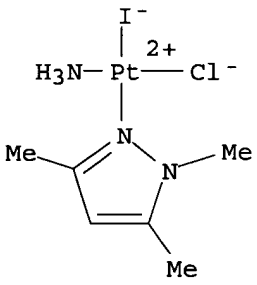
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2001094969 A5 20020415 AU 2001-94969 20011002
PRIORITY APPLN. INFO.: US 2000-678595 A 20001004
WO 2001-US30838 W 20011002

IT **406161-68-0P 406161-69-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; for prepn. of amminedichloro(N-heterocycle)platinum(II) complex)

RN 406161-68-0 CAPLUS
CN Platinum, amminechloro(3,5-dimethyl-1H-pyrazole-.kappa.N2)iodo- (9CI) (CA INDEX NAME)

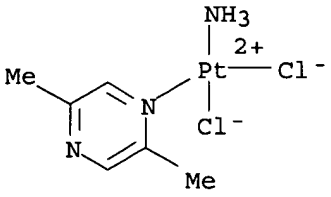


RN 406161-69-1 CAPLUS
CN Platinum, amminechloroiodo(1,3,5-trimethyl-1H-pyrazole-.kappa.N2)- (9CI) (CA INDEX NAME)

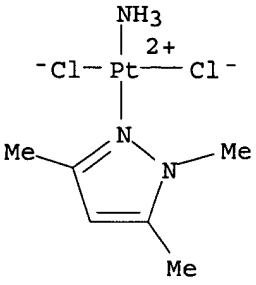


IT **301299-27-4P 406161-57-7P 406161-58-8P**
406161-60-2P 406161-62-4P 406161-63-5P
406161-64-6P 406161-65-7P 406161-66-8P
406161-67-9P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn., aq. soly., and antitumor activity)

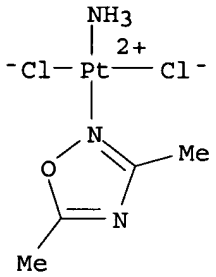
RN 301299-27-4 CAPLUS
CN Platinum, amminedichloro(2,5-dimethylpyrazine-.kappa.N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



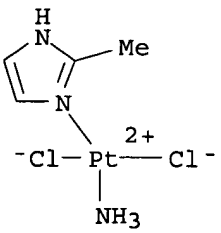
RN 406161-57-7 CAPLUS
CN Platinum, amminedichloro(1,3,5-trimethyl-1H-pyrazole-.kappa.N2)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 406161-58-8 CAPLUS
CN Platinum, amminedichloro(3,5-dimethyl-1,2,4-oxadiazole-.kappa.N2)-, (SP-4-3)- (9CI) (CA INDEX NAME)

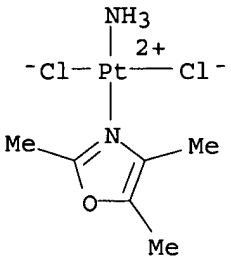


RN 406161-60-2 CAPLUS
CN Platinum, amminedichloro(2-methyl-1H-imidazole-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)

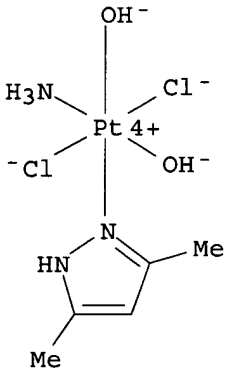


RN 406161-62-4 CAPLUS

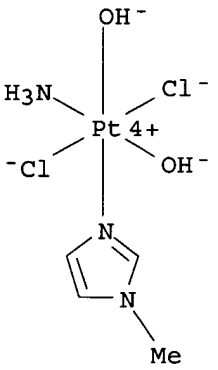
CN Platinum, amminedichloro(trimethyloxazole-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



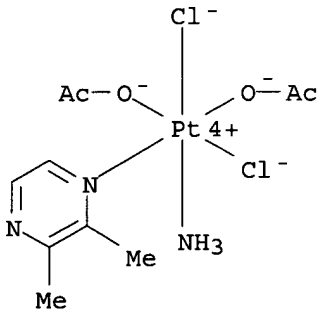
RN 406161-63-5 CAPLUS
CN Platinum, amminedichloro(3,5-dimethyl-1H-pyrazole-.kappa.N2)dihydroxy-, (OC-6-43)- (9CI) (CA INDEX NAME)



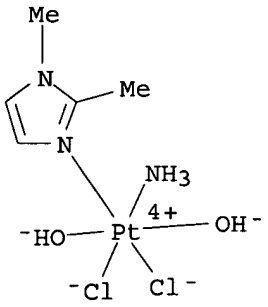
RN 406161-64-6 CAPLUS
CN Platinum, amminedichlorodihydroxy(1-methyl-1H-imidazole-.kappa.N3)-, (OC-6-43)- (9CI) (CA INDEX NAME)



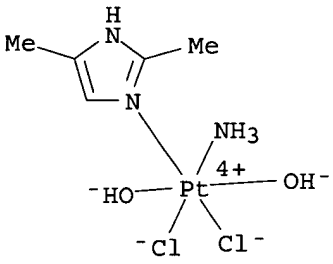
RN 406161-65-7 CAPLUS
CN Platinum, bis(acetato-.kappa.O)amminedichloro(2,3-dimethylpyrazine-.kappa.N1)-, (OC-6-43)- (9CI) (CA INDEX NAME)



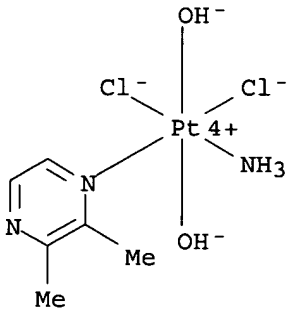
RN 406161-66-8 CAPLUS
CN Platinum, amminedichloro(1,2-dimethyl-1H-imidazole-.kappa.N3)dihydroxy-, (OC-6-43)- (9CI) (CA INDEX NAME)



RN 406161-67-9 CAPLUS
CN Platinum, amminedichloro(2,5-dimethyl-1H-imidazole-.kappa.N3)dihydroxy-, (OC-6-43)- (9CI) (CA INDEX NAME)

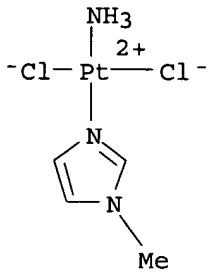


IT **301299-34-3P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn., conversion to diacetato deriv., and use as antitumor agent)
RN 301299-34-3 CAPLUS
CN Platinum, amminedichloro(2,3-dimethylpyrazine-.kappa.N1)dihydroxy-, (OC-6-43)- (9CI) (CA INDEX NAME)

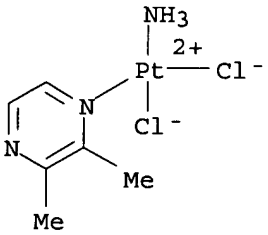


IT **114487-38-6P 301299-38-7P 406161-56-6P**
406161-59-9P 406161-61-3P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(prepn., peroxide oxidn. to dihydroxo deriv., aq. soly., and antitumor activity)

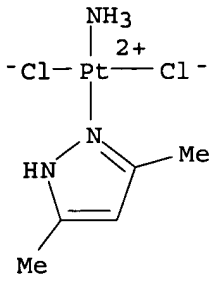
RN 114487-38-6 CAPLUS
CN Platinum, amminedichloro(1-methyl-1H-imidazole-.kappa.N3)-, (SP-4-3)-(9CI) (CA INDEX NAME)



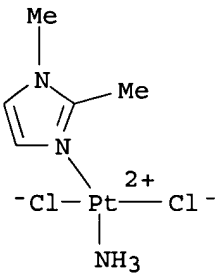
RN 301299-38-7 CAPLUS
CN Platinum, amminedichloro(2,3-dimethylpyrazine-.kappa.N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



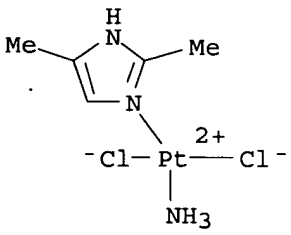
RN 406161-56-6 CAPLUS
CN Platinum, amminedichloro(3,5-dimethyl-1H-pyrazole-.kappa.N2)-, (SP-4-3)-(9CI) (CA INDEX NAME)



RN 406161-59-9 CAPLUS
CN Platinum, amminedichloro(1,2-dimethyl-1H-imidazole-.kappa.N3)-, (SP-4-3)-
(9CI) (CA INDEX NAME)



RN 406161-61-3 CAPLUS
CN Platinum, amminedichloro(2,5-dimethyl-1H-imidazole-.kappa.N3)-, (SP-4-3)-
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The invention provides a method for enhancing the water soly. of cytotoxic trans-platinum complexes. The present invention also provides a method for killing tumor cells, and a method for the treatment of tumors by the administration of a cytotoxic platinum coordination complex SP-4-2-[PtX(L)(L')(B)]+. Thus, trans-[PtCl(9-EtGua)(NH3)2]NO3 (9-EtGua = 9-ethylguanine) and trans-[PtCl(DMSO)(py)2]NO3 were prepd. and their cytotoxic properties examd.

ACCESSION NUMBER: 2002:151536 CAPLUS
DOCUMENT NUMBER: 136:193270
TITLE: Preparation of water soluble transplatinum sulfoxide and nucleobase complexes as cytotoxic and anticancer agents
INVENTOR(S): Farrell, Nicholas
PATENT ASSIGNEE(S): Virginia Commonwealth University, USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

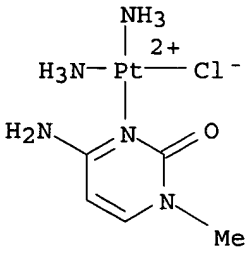
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6350740	B1	20020226	US 2000-654882	20000905
WO 2002020027	A1	20020314	WO 2001-US27387	20010905

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001087059	A5	20020322	AU 2001-87059	20010905
PRIORITY APPLN. INFO.:			US 2000-654882 A	20000905
			WO 2001-US27387 W	20010905

IT **142904-21-0P 142904-22-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of water sol. platinum nucleobase and sulfoxide complexes as anticancer agents)

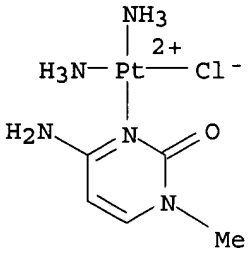
RN 142904-21-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 142904-22-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-
.kappa.N3)diamminechloro-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

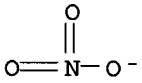
CM 1

CRN 142904-21-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

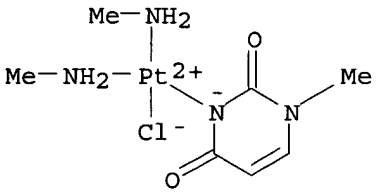
ANSWER 8 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. and crystal structure is described for trans,trans,trans-[(NH3)2Pt(N7-eade-N1)2{(MeNH2)2Pt(mura-N3)}2](ClO4)4.cntdot.4H2O (eade = 9-ethyladenine, mura = 1-methyluracilate). The combination of electronic effects (Pt(II) binding to N7 and N1) and a favorable conformation permitting efficient stabilization of the anion brings about a 109 fold increase in the exocyclic amino group acidity of 9-ethyladenine.

ACCESSION NUMBER: 2001:751965 CAPLUS
DOCUMENT NUMBER: 136:111656
TITLE: Extreme (109) acidification of adenine-NH2 in an open platinated nucleobase quartet. A pH switch with potential as a biological acid/base catalyst
AUTHOR(S): Lueth, Marc S.; Willermann, Michael; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, 44221, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (20), 2058-2059
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **388575-67-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of platinum(II) ethyladenine methyluracilate trinuclear complex)

RN 388575-67-5 CAPLUS
CN Platinum, chlorobis(methanamine)(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Replacement of one of the chloride leaving groups in trans-[PtCl2(NH3)(L)] by the nucleobase 9-ethylguanine gives the nucleobase cations [SP-4-2]-[PtCl(9-ethylguanine)(NH3)(L)]+ (L = NH3, 1; L = quinoline, 3), which are models for the monofunctional adduct on DNA. Displacement of Cl- in 1 and 3 by either 5'-guanosine monophosphate (5'-GMP) or N-acetyl-L-methionine (N-AcMet) showed clear kinetic preference for the sulfur (estd. half-lives of 1.5 and 4 h with N-AcMet against 7 and 17 h for 5'-GMP for 1 and 3, resp.). To further examine the kinetic preference, 1-methylcytosine (1-MeCyt) analogs were prepd., [SP-4-2]-[PtCl(1-MeCyt)(NH3)(L)]+ (L = NH3, 2; L = quinoline, 4). The 1-MeCyt compds., 2 and 4, resulted in slower rates of substitution by both 5'-GMP and N-AcMet in comparison to 1 and 3 (estd. half-lives for N-AcMet of 5 and 13.5 h and for 5'-GMP of 6 and 14 h for 2 and 4, resp.). Interestingly in this case, however, no selectivity for the sulfur site was obsd., a possible explanation being that mol. recognition across the square plane enhances the rate of reaction with 5'-GMP. The affinity of 3 towards S-donor ligands was exploited to remove zinc from the zinc-finger site of the C-terminal finger of the HIV-nucleocapsid protein, NCp7. The ability to eject zinc further suggested the biol. antiviral application of [SP-4-2]-[PtCl(nucleobase)(NH3)(L)]+. A preliminary survey against HIV and herpes viruses indeed showed encouraging results with some antiviral specificity, dependent on the exact nature of the compd. The initial results suggest consideration of [SP-4-2]-[PtCl(nucleobase)(NH3)(L)]+ as a novel antiviral chemotype.

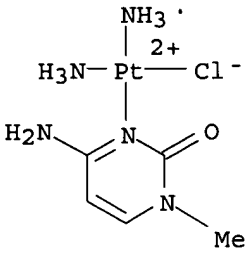
ACCESSION NUMBER: 2000:825778 CAPLUS
DOCUMENT NUMBER: 134:110107
TITLE: Modulation of the chemical and biological properties of trans platinum complexes: monofunctional platinum complexes containing one nucleobase as potential antiviral chemotypes
AUTHOR(S): Sartori, David A.; Miller, Bernhard; Bierbach, Ulrich; Farrell, N.
CORPORATE SOURCE: Department of Chemistry, Virginia Commonwealth University, Richmond, VA, 23284-2006, USA
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (2000), 5(5), 575-583
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **142904-22-1P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(modulation of chem. and biol. properties of trans-platinum complexes: monofunctional platinum complexes contg. one nucleobase as potential antiviral chemotypes)

RN 142904-22-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

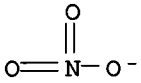
CM 1

CRN 142904-21-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 87 CAPLUS COPYRIGHT 2003 ACS

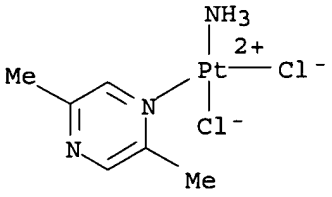
AB The present invention relates to the area of Pt amine drugs. In particular, it relates to an improved process for prepg. Pt complexes PtA2LL1 (Ia) or PtA2Y2LL1 (Ib), comprising: (1a) a 1st step, wherein [PtA4]2-, preferably PtCl42-, is reacted with L under appropriate conditions in a 1st solvent to form [PtA3(L)]-; (1b) a 2nd step, wherein [PtA3(L)]- is reacted with L' under appropriate conditions in a 2nd solvent to form cis-[PtA2(L')(L)]; (1c) in the case there Y is halogen or hydroxy a third step, wherein cis-[PtA2(L')(L)] is reacted with H2O2, Y2 or halogen contg. oxidant to form c,t,c-[PtA2Y2(L')(L)]; in the case where Y is carboxylate, carbamate or carbonate ester a 4th step, wherein an intermediate, where Y is hydroxy formed in step (1c), is functionalized with an appropriate acylating agent; and (1d) in the case where A is not a halide or is different from the original halide, addnl. step(s) in which the original halide A of an intermediate formed in step 1a or 1b, 1c or 1d is converted to a different halide or a new leaving group(s) A such as mono-dentate hydroxy, alkoxy, carboxylate or bidentate carboxylate, phosphonocarboxylate, diphosphonate, or sulfate; wherein L = amine or NH3, L' = amine but not NH3 and Y is a halogen, hydroxide, carboxylate, carbamate or carbonate ester. For example, K2[PtCl4] in N-methylpyrrolidinone reacted with 2-picoline (pic) to give K[PtCl3L] which in aq. soln. in presence of KCl reacted with NH4OAc in presence of NH4OH to give [PtCl2(NH3)(pic)]. [PtCl2(NH3)(pic)] was oxidized by H2O2 to give to give cis,trans,cis-[PtCl2(OH)2(NH3)(pic)] which was converted to [PtCl(OH)3(NH3)(pic)] and subsequently to [PtCl(OAc)3(NH3)(pic)].

ACCESSION NUMBER: 2000:742103 CAPLUS
DOCUMENT NUMBER: 133:304927
TITLE: Process for preparing amine platinum complexes
INVENTOR(S): Wong, Ernest S. Y.; Giandomenico, Christen M.
PATENT ASSIGNEE(S): Anormed, Inc., Can.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

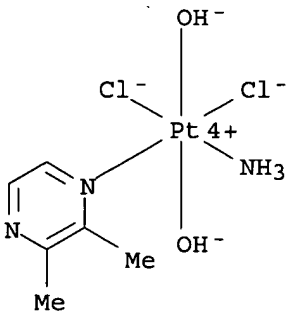
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061590	A1	20001019	WO 2000-CA385	20000411
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000009780	A	20020102	BR 2000-9780	20000411
EP 1165576	A1	20020102	EP 2000-918620	20000411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002541263	T2	20021203	JP 2000-610861	20000411
EE 200100536	A	20030217	EE 2001-536	20000411
NO 2001004957	A	20011203	NO 2001-4957	20011012
BG 106090	A	20020628	BG 2001-106090	20011108

PRIORITY APPLN. INFO.: US 1999-128939P P 19990413
WO 2000-CA385 W 20000411
OTHER SOURCE(S): MARPAT 133:304927

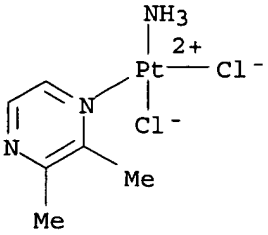
IT **301299-27-4P 301299-34-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(improved prepn. of antitumor agent)
RN 301299-27-4 CAPLUS
CN Platinum, amminedichloro(2,5-dimethylpyrazine-.kappa.N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 301299-34-3 CAPLUS
CN Platinum, amminedichloro(2,3-dimethylpyrazine-.kappa.N1)dihydroxy-, (OC-6-43)- (9CI) (CA INDEX NAME)



IT **301299-38-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for improved prepn. of platinum amine complexes as antitumor agents)
RN 301299-38-7 CAPLUS
CN Platinum, amminedichloro(2,3-dimethylpyrazine-.kappa.N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 11 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Three complexes of model nucleobases with exocyclic oxygen atoms (1-methyluracilate, mura; 1-methylcytosine, mcyt; 9-methylguanine, Hmgua) which contain PtII bonded to a ring N atom and an alkali metal ion (Cs+, K+, Na+) bonded to a keto oxygen of the bases, trans-Cs[Pt(NH3)(mura)I2].cntdot.4H2O (1), trans-K[Pt(NH3)2(mcyt)2][PF6]3.cntdot.H2O (2), and trans-[Pt(NH3)(Hmgua)2(mcyt)Na(H2O)2][ClO4]3.cntdot.0.5H2O (3), were prepd. and their crystal structures detd. The compds. were studied, among others, with regard to the role of alkali metal ions for the rotation of nucleobases when bound to PtII. While in the case of 1 the alkali metal ion is necessary for charge compensation and for this reason its binding to the platinated mura is not fully unexpected, it is surprising to see that alkali metal ions even bind to cationic complexes of PtII contg. neutral nucleobases (2, 3).

ACCESSION NUMBER: 2000:691638 CAPLUS
DOCUMENT NUMBER: 134:80093
TITLE: Exocyclic oxygen atoms of platinated nucleobases as binding sites for alkali metal ions
AUTHOR(S): Freisinger, Eva; Schneider, Alexandra; Drumm, Markus; Hegmans, Alexander; Meier, Susanne; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: Dalton (2000), (19), 3281-3287
CODEN: DALTFG
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **315662-46-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure)

RN 315662-46-5 CAPLUS

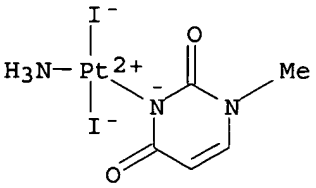
CN Cesium(1+), diaqua-, (SP-4-1)-amminediiodo(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)platinate(1-), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 315662-45-4
CMF C5 H8 I2 N3 O2 Pt . Cs H4 O2

CM 2

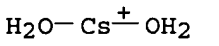
CRN 315662-44-3
CMF C5 H8 I2 N3 O2 Pt
CCI CCS



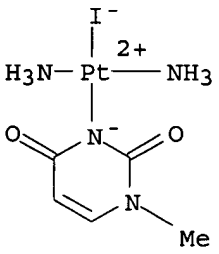
CM 3

CRN 81009-40-7

CMF Cs H4 O2
CCI CCS



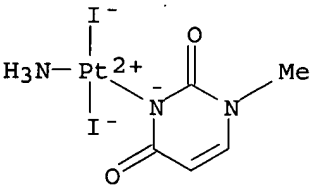
IT **103439-49-2P 315662-52-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 103439-49-2 CAPLUS
CN Platinum, diammineiodo(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 315662-52-3 CAPLUS
CN Platinum(2+), tetraammine-, (SP-4-1)-, bis[(SP-4-1)-amminediiodo(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)platinate(1-)] (9CI) (CA INDEX NAME)

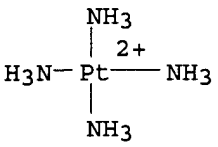
CM 1

CRN 315662-44-3
CMF C5 H8 I2 N3 O2 Pt
CCI CCS

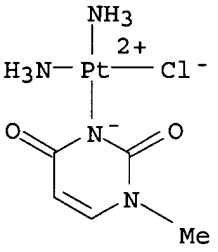


CM 2

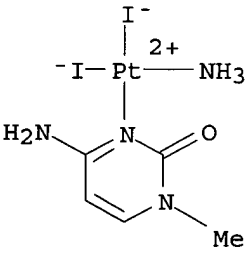
CRN 16455-68-8
CMF H12 N4 Pt
CCI CCS



IT **85715-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of cesium platinum ammine methyluracilate complex)
RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **161269-39-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of sodium platinum ammine methylcytosine methylguanine complex)
RN 161269-39-2 CAPLUS
CN Platinum, (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)amminediiodo-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 87 CAPLUS COPYRIGHT 2003 ACS

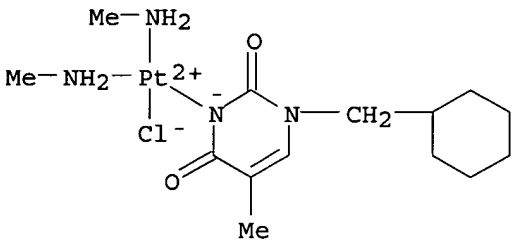
AB Solid phase synthesis of oligodeoxyribonucleotide complex platinum is reported.

ACCESSION NUMBER: 2000:76526 CAPLUS
DOCUMENT NUMBER: 132:265426
TITLE: Solid-phase synthesis of a monofunctional trans-a2Pt11 complex tethered to a single-stranded oligonucleotide
AUTHOR(S): Schmidt, Kathrin S.; Filippov, Dmitri V.; Meeuwenoord, Nico J.; Van der Marel, Gijs; Van Boom, Jacques H.; . Lippert, Bernhard; Reedijk, Jan
CORPORATE SOURCE: Leiden Inst. Chem., Gorlaeus Lab., Leiden Univ., Leiden, 2300 RA, Neth.
SOURCE: Angewandte Chemie, International Edition (2000), 39(2), 375-377
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:265426

IT **263257-48-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid-phase synthesis of a monofunctional trans-a2Pt11 complex tethered to a single-stranded oligonucleotide)

RN 263257-48-3 CAPLUS

CN Platinum, chloro[1-(cyclohexylmethyl)-5-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3]bis(methanamine)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 13 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Trans-[Pt(CH3NH2)2(1-MeC-N4)2]X2 (3a, X = NO3-; 3b, X = ClO4-), contg. the model nucleobase 1-methylcytosine (1-MeC) platinated at N4 and protonated at N3, hence in its rare tautomeric form, was prepd. from the PtIV precursor trans,trans,trans-[Pt(CH3NH2)2(1-MeC-N4)2(OH)2](NO3)2.cntdot.2H2O (2) upon redn. with H2. Crystn. of 3a from 1 M NaOH afforded trans-[Pt(CH3NH2)2(1-MeC--N4)2].cntdot.4H2O (4a) or, following lyophilization and deprotonation in CH3OH by Me3CONa, gave trans-[Pt(CH3NH2)2(1-MeC--N4)2].cntdot.2CH3OH (4b). While dihedral angles between the coplanar bases and the PtN4 planes are large in the case of 2 (84.8(1).degree.) and 3b (73.9(1).degree.), they become markedly smaller in 4a (55.5(2).degree.) and 4b (26.6(2).degree.) as a consequence of pairwise intramol. H bonding between the NH protons of the CH3NH2 groups and the N3 positions of the cytosine nucleobases. DFT calcns. for the corresponding NH3 complex gave a dihedral angle of 22.3.degree.. The switch of the mutually trans-oriented ligand pairs from approx. perpendicular to roughly coplanar appears to take place during the crystn. process, probably because of competition between intramol. H bonding and intermol. H bonding with the solvent. Crystal data: 2, triclinic, space group P.hivin.1, a 5.937(1), b 8.228(2), c 12.470(2) .ANG., .alpha. 80.36(3), .beta. 80.80(3), .gamma. 80.54(3).degree., Z = 2; 3b, triclinic, P.hivin.1, a 7.392(1), b 9.072(2), c 10.047(2) .ANG., .alpha. 112.40(3), .beta. 106.07(3), .gamma. 94.66(3).degree., Z = 2; 4a, triclinic, P.hivin.1, a 7.104(1), b 7.549(2), c 9.209(2) .ANG., .alpha. 87.74(3), .beta. 88.04(3), .gamma. 85.92(3).degree., Z = 2; 4b, triclinic, P.hivin.1, a 7.045(1), b 7.421(1), c 9.966(2) .ANG., .alpha. 109.25(3), .beta. 99.22(3), .gamma. 95.02(3).degree., Z = 2.

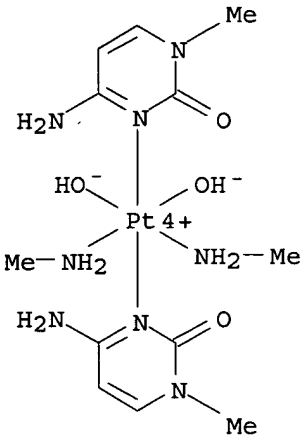
ACCESSION NUMBER: 1999:346517 CAPLUS
DOCUMENT NUMBER: 131:110357
TITLE: A Major, pH-Induced Stereochemical Switch of Pairs of trans-Oriented Ligands in Complexes of trans-a2PtII (a = NH3, CH3NH2)
AUTHOR(S): Mueller, Jens; Glahe, Frank; Freisinger, Eva; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, D-44221, Germany
SOURCE: Inorganic Chemistry (1999), 38(13), 3160-3166
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **230622-36-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and isomerization in study of pH induced stereochem. switch)

RN 230622-36-3 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)dihydroxybis(methanamine)-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

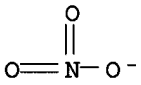
CM 1

CRN 230622-35-2
CMF C12 H26 N8 O4 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 14 OF 87 CAPLUS COPYRIGHT 2003 ACS

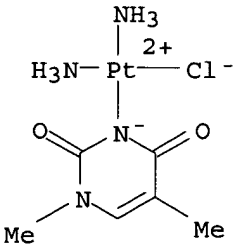
AB The x-ray structure of the compd. described as trans-[(NH3)2Pr(9-MeA-N7)2](ClO4)2.cntdot.H2O (3c) is actually that of trans-[(NH3)2Pt(9-MeAH-N7)2](ClO4)4.cntdot.2H2O (3a). Formulas in the abstr. (line 2), the Exptl. Section (page 4125, right column, line 67), the caption of Figure 5, and headings of Tables 1 and 3 should be altered accordingly. Entries in Table 1 should be changed as follows: compd. 3a, C12H26Cl4N12O18Pt, formula wt. 963.305, .rho.calcd 2.030. Supporting Information is available free of charge via the Internet at http://pubs.acs.org; this includes Figure S8, packing diagram of 3a, and Tables S2, S4, and S6 giving the crystal data, exptl. conditions, and details of refinement, anisotropic displacement coeffs., and at. coordinates and equiv. isotropic displacement coeffs. for 3a (PDF).

ACCESSION NUMBER: 1999:173741 CAPLUS
DOCUMENT NUMBER: 131:12910
TITLE: Bis(purine) Complexes of trans-a2PtII: Preparation and X-ray Structures of Bis(9-methyladenine) and Mixed 9-Methyladenine, 9-Methylguanine Complexes and Chemistry Relevant to Metal-Modified Nucleobase Triples and Quartets. [Erratum to document cited in CA124:330618]
AUTHOR(S): Schreiber, Andre; Lueth, Marc S.; Erxleben, Andrea; Fusch, Edda C.; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, D-44221, Germany
SOURCE: Journal of the American Chemical Society (1999), 121(13), 3248
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149951-64-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum amine purine base complex (Erratum))

RN 149951-64-4 CAPLUS

CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



ANSWER 15 OF 87 CAPLUS COPYRIGHT 2003 ACS

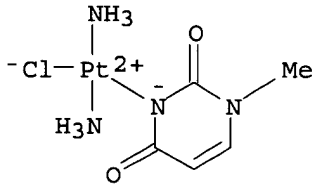
AB Trans-[Pt(NH3)2(mura)2] 1 (mura = 1-methyluracilate), a compd. of very low water soly., is markedly solubilized in the presence of acid or suitable metal salts due to protonation and metal binding to the exocyclic O atoms, resp. The perchlorate salt trans-[Pt(NH3)2(Hmura)2][ClO4]2.cntdot.2H2O 2 was characterized by x-ray anal. With Ag+, 1 formed heteronuclear species of varying stoichiometries, e.g. Pt2Ag3 3, the compn. of which can be further varied by the presence of alkali metal salts. Trans-[{Pt(NH3)2(mura)2}2AgNa(H2O)4][ClO4]2.cntdot.6.5H2O 4 appears to be the 1st structurally characterized example of a nucleobase complex contg. three different metal ions. Tetranuclear cations of 4 are arranged in the crystal in such a way as to permit both intermol. H bonding between NH3 ligands and O2 sites of mura nucleobases and .pi. stacking between adjacent trans-[Pt(NH3)2(mura)2] entities. This feature is radically different from that obsd. in related di- and tri-nuclear complexes derived from cis-(am)2PtII. With Hg(II) salts, initial binding to exocyclic O atoms of the mura ligand takes place, followed by metal binding to the C5 atoms of both uracil ligands of 1.

ACCESSION NUMBER: 1999:14033 CAPLUS
DOCUMENT NUMBER: 130:245563
TITLE: Crystal structures of a protonated form of trans-[Pt(NH3)2(mura)2] and of a derivative containing three different metal ions, Pt2+, Ag+, and Na+ (mura = 1-methyluracilate). Major difference in packing between heteronuclear pyrimidine nucleobase complexes of cis- and trans-(NH3)2PtII
AUTHOR(S): Zamora, Felix; Witkowski, Holger; Freisinger, Eva; Muller, Jens; Thormann, Birgit; Albinati, Alberto; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (2), 175-182
CODEN: JCDTBI; ISSN: 0300-9246
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **220760-69-0**, trans-Diammine(chloro)(methyluracilato)platinum
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum-silver methyluracilate trinuclear complex)

RN 220760-69-0 CAPLUS

CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

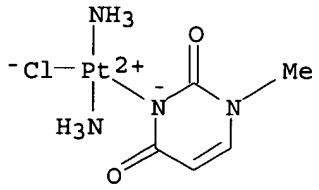
ANSWER 16 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. of a cyclic arrangement of the four model nucleobases 1-methyluracilate (mura), 9-ethyladenine (eade), 9-ethylguanine (Hegua) and 1-methylcytosine (mcyt), held together by two metal entities [trans-(NH3)2PtII and trans-(MeNH2)2PtII] and multiple H bond interactions in trans,trans-[(NH3)2Pt(mura-N3)(eade-N7,N1)Pt(MeNH2)2(Hegua-N7).cntdot.myct]2 [myct.cntdot.Hmyct] (ClO4)4.5 (NO3)2.5 is reported.

ACCESSION NUMBER: 1998:815735 CAPLUS
DOCUMENT NUMBER: 130:204186
TITLE: Combining four different model nucleobases (uracil, adenine, guanine, cytosine) via metal binding and H bond formation in a single compound
AUTHOR(S): Sigel, Roland K. O.; Thompson, Susan M.; Freisinger, Eva; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: Chemical Communications (Cambridge) (1999), (1), 19-20
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **220760-69-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for prepn. of platinum amine complexed with uracil, adenine, guanine, and cytosine via metal binding and H bond formation)

RN 220760-69-0 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 17 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Reaction of a PtII complex contg. two 1-methylcytosine (1-MeC) nucleobases bound through the exocyclic amino group N4, trans-[Pt(NH3)2(1-MeC-N4)2](NO3)2 (1), with the heterometal species [(dien)Pd]2+ or Hg2+ gives trans-[(NH3)2Pt[(N4-1-MeC--N3)Pd(dien)]2](ClO4)4.cntdot.2H2O (3) and trans-[(NH3)2Pt(N4-1-MeC--N3)2Hg](NO3)2.cntdot.2H2O (4), resp. The heterometals are bound through the N3 positions of the two cytosine rings. 1 Contains the nucleobase as its rare iminooxo tautomer. In the solid-state structure of 1, the two nucleobases display a syn orientation between Pt and the endocyclic N3 position, whereas in 3 they adopt an anti conformation. In both compds. the cytosine bases are in a head-to-tail orientation. In the bimetallic 4 however, the 1-methylcytosine ligands are head-to-head and syn with the two nucleobases acting as chelating ligands. The Pt-Hg distance in 4 is quite short (2.7498(6) .ANG.), suggesting a weak bonding interaction. In 3 the Pt-Pd distance (5.13 .ANG.) is too long for any interaction. While H-bond formation between the iminooxo tautomer of 1-MeC in 1 with free 1-MeC and likewise between the deprotonated form trans-[Pt(NH3)2(1-MeC--N4)2] (2) and free 9-ethylguanine (9-EtGH) is possible only if the cytosine bases are in an anti orientation, there is no indication for such H-bonding patterns from 1H NMR studies.

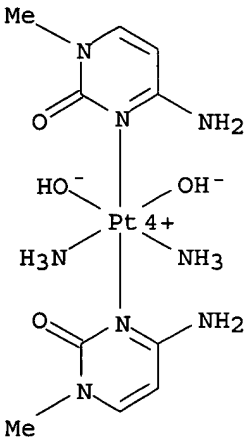
ACCESSION NUMBER: 1998:223265 CAPLUS
DOCUMENT NUMBER: 128:303325
TITLE: Metal-Stabilized rare tautomers of nucleobases. Part 7. Affinity of the iminooxo tautomer anion of 1-methylcytosine in trans-[Pt(NH3)2(1-MeC-N4)2]2+ for heterometals
AUTHOR(S): Muller, Jens; Zangrando, Ennio; Pahlke, Norbert; Freisinger, Eva; Randaccio, Lucio; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: Chemistry--A European Journal (1998), 4(3), 397-405
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **101152-06-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of)

RN 101152-06-1 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminedihydroxy-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

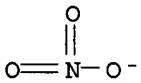
CM 1

CRN 101152-05-0
CMF C10 H22 N8 O4 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

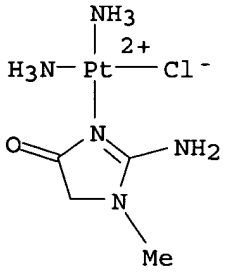
L7 ANSWER 18 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Cisplatin is an extremely effective cancer chemotherapeutic agent, but its use is often accompanied by toxicity. Second generation drugs such as carboplatin are becoming more widely used because of reduced toxicity. Since biotransformation products have been implicated in the toxic responses, the authors have begun to investigate the reactions of cisplatin and carboplatin with potential biol. ligands. Reaction products were characterized using HPLC with inductively coupled plasma-mass spectrometry (HPLC-ICP-MS), 1H and 13C NMR and fast atom bombardment-mass spectrometry (FAB-MS). Three Pt-creatinine complexes, cis-[Pt(NH3)2Cl(Creat)]+, cis-[Pt(NH3)2(H2O)(Creat)]2+ and cis-[Pt(NH3)2(Creat)2]2+, were synthesized and the platinum was shown to coordinate to the ring nitrogen, N(3). Human urine samples from patients on cisplatin chemotherapy were shown to contain cisplatin, its hydrolysis product and biotransformation products contg. Pt-creatinine, Pt-urea and Pt-uric acid complexes. Urine from carboplatin patients shows fewer biotransformation products. Studies with control and diabetic (protected against cisplatin toxicity) rats showed systematic differences in the biotransformation products formed on administration of cisplatin.

ACCESSION NUMBER: 1997:504528 CAPLUS
DOCUMENT NUMBER: 127:199565
TITLE: Determination of biotransformation products of platinum drugs in rat and human urine
AUTHOR(S): Tang, Xia; Hayes, Jerry W., II; Schroder, Louis; Cacini, William; Dorsey, John; Elder, R. C.; Tepperman, Katherine
CORPORATE SOURCE: Barrett Center for Cancer Prevention, Treatment and Research, Cincinnati, OH, 45267, USA
SOURCE: Metal-Based Drugs (1997), 4(2), 97-109
CODEN: MBADEI; ISSN: 0793-0291
PUBLISHER: Freund
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **194796-95-7**
RL: BSU (Biological study, unclassified); FMU (Formation, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(detn. of biotransformation products of platinum drugs in rat and human urine using HPLC-MS in relation to reaction with creatinine and toxicity and diabetes)

RN 194796-95-7 CAPLUS
CN Platinum(1+), (2-amino-1,5-dihydro-1-methyl-4H-imidazol-4-one-.kappa.N3)diamminechloro-, (SP-4-3)- (9CI) (CA INDEX NAME)

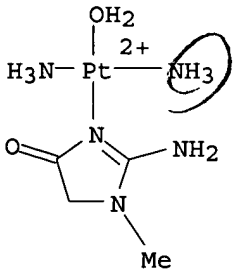


IT **135390-29-3**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(detn. of biotransformation products of platinum drugs in rat and human

urine using HPLC-MS in relation to reaction with creatinine and toxicity and diabetes)

RN 135390-29-3 CAPLUS

CN Platinum(2+), (2-amino-1,5-dihydro-1-methyl-4H-imidazol-4-one-N3)diammineaqua-, (SP-4-3)- (9CI) (CA INDEX NAME)



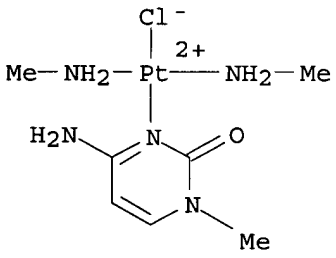
ANSWER 19 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The analogy between H-bonded nucleobase pairs and their metalated analogs is extended to the hemiprotonated pair of 7,9-dimethylguanine (7,9-DimeG) and the Watson-Crick and reversed Watson-Crick pair between 7,9-dimethylguaninium (7,9-DimeGH+) and 1-methylcytosine (1-MeC). The crystal structure analyses of two model compds., trans-[Pt(CH3NH2)2(7,9-DimeG-N1)2](NO3)2 and trans-[Pt(NH3)2(1-MeC-N3)(7,9-DimeG-N1)](PF6)2.cntdot.2.5 H2O (I) are reported. Pt binding is through N1 of 7,9-DimeG and N3 of 1-MeC. In soln., I exists in a mixt. with Watson-Crick and reversed Watson-Crick arrangements of the two bases, depending on solvent, concn. and anions.

ACCESSION NUMBER: 1997:311760 CAPLUS
DOCUMENT NUMBER: 127:50449
TITLE: Metal-modified nucleobase pairs involving 7,9-dimethylguanine: trans-a2PtII analogs (a = NH3 or CH3NH2) of Watson-Crick GC and homo GG pairs
AUTHOR(S): Metzger, Susanne; Erxleben, Andrea; Lippert, Bernhard
CORPORATE SOURCE: Abteilung Chemie, Universitat Dortmund, Dortmund, D-44221, Germany
SOURCE: JBIC, Journal of Biological Inorganic Chemistry (1997), 2(2), 256-264
CODEN: JJBCFA; ISSN: 0949-8257
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **128636-28-2P 142904-22-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and crystal structure of metal-modified nucleobase pairs involving dimethylguanine)

RN 128636-28-2 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)chlorobis(methanamine)-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



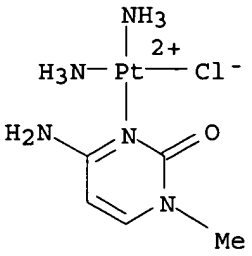
⊖ Cl⁻

RN 142904-22-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

CM 1

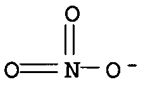
CRN 142904-21-0
CMF C5 H13 Cl N5 O Pt

CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



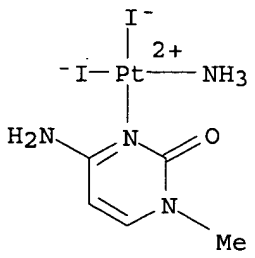
L7 ANSWER 20 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A square-planar Pt(II) complex contg. four different ligands, including the two model nucleobases 1-methylcytosine (1-MeC) and 9-ethylguanine (9-EtGH), was prepd. and studied by x-ray crystallog. [PtI(1-MeC)(9-EtGH)(NH3)]ClO4.cntdot.1.5H2O (1) crystallizes in the monoclinic system, space group C2/c with a 16.577(3), b 16.638(2), c 17.923(3) .ANG., .beta. 114.37(1).degree., Z = 8. The two nucleobases which are platinated at N3 (1-MeC) and N7 (9-EtGH) are cis to each other and oriented in a way as to form a very weak H bond (3.39 .ANG.) between NH2(4) of 1-MeC and O(6) of 9-EtGH. The guanine ligand is trans to I-. The title compd. represents one of three possible geometrical isomers of compds. having this compn. A closely related complex, cis-[PtI(1-MeC)2(NH3)]ClO4 (3), has likewise been isolated and x-ray structurally characterized: triclinic system, space group P.hivin.1 with a 10.490(4), b 10.886(4), c 9.529(3) .ANG., .alpha. 94.18(3), .beta. 106.28(3), .gamma. 106.33(3).degree., Z = 2. In 3 the two 1-MeC bases are platinated at N3 and oriented head-tail, with intramol. H bonds of 3.22 and 2.95 .ANG. between pairs of NH2(4) and O(2) groups.

ACCESSION NUMBER: 1997:295135 CAPLUS
DOCUMENT NUMBER: 126:311303
TITLE: Platinum(II) nucleobase complexes containing up to four different ligands: syntheses and x-ray structure determinations of cis-[PtI(1-MeC)2(NH3)]ClO4 and [PtI(1-MeC)(9-EtGH)(NH3)]ClO4.cntdot.1.5H2O
AUTHOR(S): Wienkotter, Thomas; Sabat, Michal; Trotscher-Kaus, Gabriele; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Univ. Dortmund, Dortmund, D-44221, Germany
SOURCE: Inorganica Chimica Acta (1997), 255(2), 361-366
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **161269-39-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum(II) nucleobase complexes contg. up to four different ligands)

RN 161269-39-2 CAPLUS
CN Platinum, (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)amminediiodo-, (SP-4-1)- (9CI) (CA INDEX NAME)



ANSWER 21 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. and x-ray crystal structure detn. of a Pt(IV) nucleobase complex, trans,trans,trans-[Pt(NH3)2(1-MeU)2(H3O2)]n(NO3)n.cntdot.(4H2O)n (1-MeU = 1-methyluracilate-N3) is reported. The compd., obtained upon recrystn. of trans,trans,trans-[Pt(NH3)2(1-MeUH)2(OH)2](NO3)2 (1-MeUH = neutral 1-methyluracil-N3) from water, crystallizes in the triclinic system, space group P.hivin.1 with two independent cations in the unit cell: a 7.3023(8), b 10.1470(20), c 13.4220(20) .ANG., .alpha. 78.800(17), .beta. 83.580(9), .gamma. 78.930(10).degree., Z = 2. Description of its solid state structure as a H3O2- compd. rather than a genuine mixed H2O,OH- complex is based on the presence of very short H bonds of 2.450(6) .ANG. between the oxygens of axial aqua and hydroxo ligands of adjacent Pt(IV) cations, leading to infinite chains.

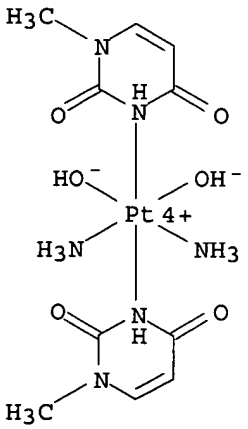
ACCESSION NUMBER: 1997:294759 CAPLUS
DOCUMENT NUMBER: 126:311299
TITLE: H3O2- bridging in a Pt(IV) nucleobase complex leading to infinite chains: trans,trans,trans-[Pt(NH3)2(1-MeU)2(H3O2)]n(NO3)n.cntdot.(4H2O)n (1-MeU = 1-methyluracilate)
AUTHOR(S): Lianza, Francesca; Albinati, Alberto; Lippert, Bernhard
CORPORATE SOURCE: Ist. Chimico Farmaceutico, Univ. Milano, Milan, I-20131, Italy
SOURCE: Inorganica Chimica Acta (1997), 255(2), 313-318
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **129700-79-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum methyluracilato ammine hydroxo aqua infinite chain complex)

RN 129700-79-4 CAPLUS
CN Platinum(2+), diamminedihydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedione-.kappa.N3)-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

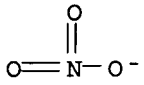
CM 1

CRN 129700-78-3
CMF C10 H20 N6 O6 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



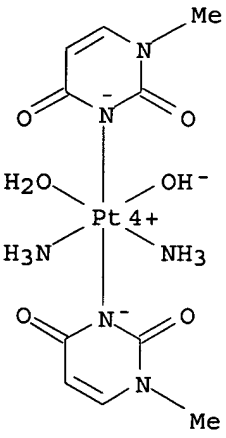
IT **189180-10-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and hydrogen bonding)
RN 189180-10-7 CAPLUS
CN Platinum(1+), diammineaquahydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (OC-6-23)-, nitrate, tetrahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 189180-09-4
CMF C10 H19 N6 O6 Pt . N O3

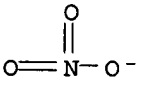
CM 2

CRN 189180-08-3
CMF C10 H19 N6 O6 Pt
CCI CCS



CM 3

CRN 14797-55-8
CMF N O3



L7 ANSWER 22 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Trans-Diammineplatinum(II), trans-(NH3)2Pt(II), forms a mixed nucleobase complex trans-[(NH3)2Pt(9-EtG-N7)(1-MeC-N3)](ClO4)2 (1) with 9-ethylguanine (9-EtGH) and 1-methylcytosine (1-MeC) and, upon deprotonation of the 9-EtGH ligand at the N1 position, trans-[(NH3)2Pt(1-MeC-N3)(9-EtG-N7)](ClO4) (2). As demonstrated by 1H NMR spectroscopy (concn. dependence, NOESY), self-complementary cations of 2 dimerize in DMSO soln. to give a dimetalated base quartet contg. six H bonds, four between pairs of guanine O(6) and cytosine NH2(4) sites and, for the 1st time, two between cytosine H(5) and the deprotonated guanine N(1) positions. This H bonding pattern extends the known base pairing between cytosine and guanine (Hoogsteen: between protonated C and neutral G; Watson-Crick: between neutral C and neutral G) by a pair between neutral C and anionic G. Metal binding to cytosine-N(3) and guanine-N(7) is a prerequisite for its formation.

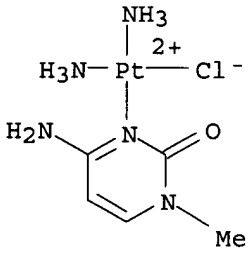
ACCESSION NUMBER: 1996:689410 CAPLUS
DOCUMENT NUMBER: 126:69225
TITLE: A Metalated Guanine,Cytosine Base Quartet with a Novel GC Pairing Pattern Involving H(5) of C
AUTHOR(S): Metzger, Susanne; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, University of Dortmund, Dortmund, D-44221, Germany
SOURCE: Journal of the American Chemical Society (1996), 118(49), 12467-12468
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **142904-22-1**, trans-Diamminechloro(1-methylcytosine)platinum(1+) nitrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum guanine cytosine ammine complexes)

RN 142904-22-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

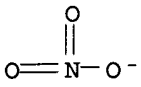
CM 1

CRN 142904-21-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



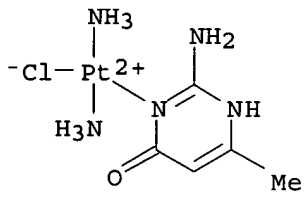
ANSWER 23 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Isomeric tri- and tetramine type complexes of Pt(II) with cytosine and isocytosine and their 6-Me and 6-fluoro derivs. were prepd. Structures of the compds. prepd. and the nature of donating ligand atoms were elucidated by TLC, conductometry, and IR and 1H NMR spectroscopy. The effect of the coordination on acidic properties of the pyrimidines were studied.

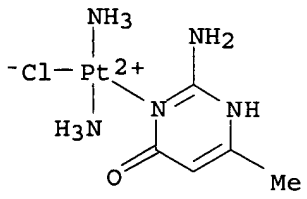
ACCESSION NUMBER: 1996:577114 CAPLUS
DOCUMENT NUMBER: 126:26001
TITLE: Mononuclear cationic complexes of platinum(II) with cytosine and isocytosine derivatives
AUTHOR(S): Yakovlev, K. I.; Lapina, S. F.; Stetsenko, A. I.; Alekseeva, G. M.
CORPORATE SOURCE: Sankt-Peterburgskii Khimiko-Farmatsevticheskii Institut, St. Petersburg, Russia
SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya (1996), 39(3), 75-79
CODEN: IVUKAR; ISSN: 0579-2991
PUBLISHER: Ivanovskaya Gosudarstvennaya Khimiko-Tekhnologicheskaya Akademiya
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **184352-49-6P 184489-79-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acid dissocn. const.)

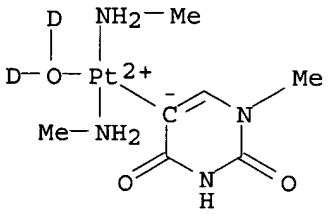
RN 184352-49-6 CAPLUS
CN Platinum(1+), (2-amino-6-methyl-4(1H)-pyrimidinone-.kappa.N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



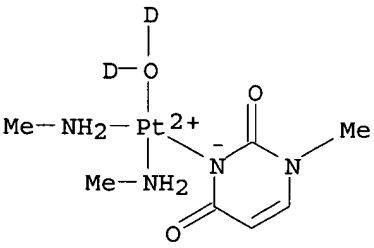
RN 184489-79-0 CAPLUS
CN Platinum(1+), (2-amino-6-methyl-4(1H)-pyrimidinone-.kappa.N3)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



~~L7~~ ANSWER 24 OF 87 CAPLUS COPYRIGHT 2003 ACS
AB The errors were not reflected in the abstr. or the index entries.
ACCESSION NUMBER: 1996:569483 CAPLUS
DOCUMENT NUMBER: 125:276130
TITLE: Uracil C(5) Position as a Metal Binding Site: Solution and X-ray Crystal Structure Studies of PtII and HgII Compounds. [Erratum to document cited in CA124:176464]
AUTHOR(S): Hoepp, Markus; Erxleben, Andrea; Rombeck, Ingo; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, 44221, Germany
SOURCE: Inorganic Chemistry (1996), 35(21), 6352
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **173776-52-8P**
RL: BYP (Byproduct); PREP (Preparation)
(formation from platinum amine uracilato and platinum amine aqua complexes (Erratum))
RN 173776-52-8 CAPLUS
CN Platinum(1+), aqua-d2-bis(methanamine)(1,2,3,4-tetrahydro-1-methyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)- (9CI) (CA INDEX NAME)

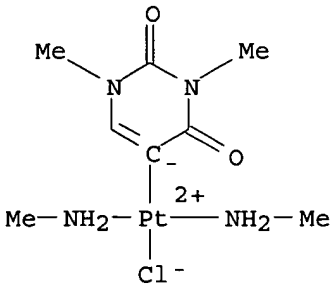


IT **173776-51-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation from platinum amine uracilato and platinum amine aqua complexes (Erratum))
RN 173776-51-7 CAPLUS
CN Platinum(1+), aqua-d2-bis(methanamine)(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **173776-38-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of (Erratum))
RN 173776-38-0 CAPLUS
CN Platinum, chlorobis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-

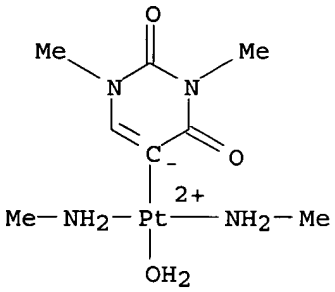
5-pyrimidinyl)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **173776-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with aq. ammonia (Erratum))
RN 173776-53-9 CAPLUS
CN Platinum(1+), aquabis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)-, perchlorate (9CI) (CA INDEX NAME)

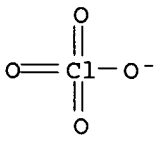
CM 1

CRN 173776-36-8
CMF C8 H19 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4

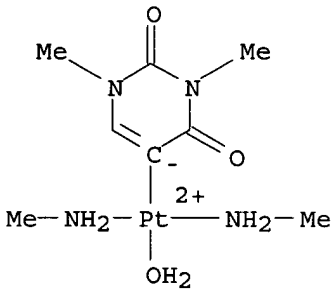


IT **173776-37-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with chloride (Erratum))

RN 173776-37-9 CAPLUS
CN Platinum(1+), aquabis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

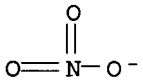
CM 1

CRN 173776-36-8
CMF C8 H19 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



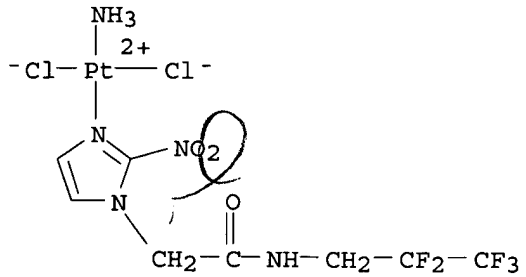
ANSWER 25 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The monoclonal antibody ELK3-51 was previously developed to detect adducts of the 2-nitroimidazole EF5. Direct immunofluorescence was used to detect adducts of EF5 or of a platinated deriv. cis-[PtCl2(NH3)EF5] in SCCVII cells treated under aerobic or hypoxic conditions. Fluorescence measurements of these cells using both image and flow cytometric methods were compared, giving similar profiles. Platination significantly decreased immunofluorescence levels (.apprx.4-fold less than EF5) after 3 h in hypoxia, but also increased levels after exposure in air (.apprx.1.5 .times.) such that the hypoxic ratio decreased from .apprx.50 to .apprx.13. Platinated EF5 also showed significantly greater cytotoxicity than its parent in both aerobic and hypoxic cells. These results are consistent with targeting of EF5 to DNA, which was confirmed qual. by confocal microscopy.

ACCESSION NUMBER: 1996:492707 CAPLUS
DOCUMENT NUMBER: 125:185094
TITLE: Immunocytochemical labeling of aerobic and hypoxic mammalian cells using a platinated derivative of EF5
AUTHOR(S): Matthews, J.; Adomat, H.; Farrell, N.; King, P.; Koch, C.; Lord, E.; Palcic, B.; Poulin, N.; Sangulin, J.; Skov, K.
CORPORATE SOURCE: Department Medical Biophysics, BC Cancer Research Centre, Vancouver, BC, V5Z 1L3, Can.
SOURCE: British Journal of Cancer, Supplement (1996), 74(27), S200-S203
CODEN: BJCSB5; ISSN: 0306-9443
PUBLISHER: Stockton
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **180990-37-8**
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(immunocytochem. labeling of aerobic and hypoxic mammalian cells using a platinated deriv. of EF5)

RN 180990-37-8 CAPLUS
CN Platinum, amminedichloro[2-nitro-N-(2,2,3,3,3-pentafluoropropyl)-1H-imidazole-1-acetamide-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



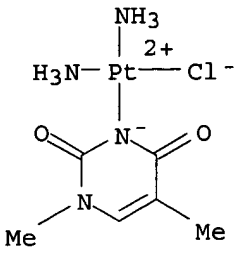
L7 ANSWER 26 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Mononuclear bis(purine) complexes of trans-a2PtII, trans-[(NH3)2Pt(9-MeA-N7)(9-MeGH-N7)](NO3)2.cntdot.H2O (1b) (9-MeA = 9-methyladenine; 9-MeGH = 9-methylguanine) and trans-[(NH3)2Pt(9-MeA-N7)2](ClO4)2.cntdot.H2O (3c), were prepd. and their structures detd. by x-ray crystallog. 1B: Space group P.hivin.1, a 7.245(5) .ANG., b 7.715(6), c 10.907(8) .ANG., .alpha. 82.36(6), .beta. 86.62(6), .gamma. 70.15(6).degree., V = 568.3(7) .ANG.3, Z = 1. 3C: Space group P21/c, a 8.312(2), b 15.386(3), c 12.365(2) .ANG., .beta. 94.83(3).degree., V = 1575.72(55) .ANG., Z = 2. The cation of 3c is centrosym. In the cation of 1b, the two purines adopt a head-head orientation with an intramol. H bond of 2.94(3) .ANG. between the exocyclic amino group of 9-MeA and the exocyclic carbonyl group of 9-MeGH. Di- and trinuclear derivs. of 1b and 3c were synthesized and/or studied in soln. They include compds. ClZ(N1-A-N7)Z(GH) (2a), TZ(N1-A-N7)Z(GH) (2b), (GH)Z(N1-A-N7)(T) (2c), and (GH.bul.N7)(A-N1)Z(N1-A-N7)Z(GH) (2d) as well as XZ(N1-A-N7)Z(N7-A-N1)ZX (X = Cl (4), GH (guanine) (5a), T (thymine) (5b)) with Z = trans-a2PtII entities (a = NH3 or CH3NH2), (A = adenine). The fact that Pt-(A-N1) and Pt-(A-N7) vectors are at right angles and the nucleobases essentially coplanar in many cases leads to intramol. H bonding involving NH2(6) of 9-MeA and exocyclic groups of the other nucleobases. The chem. shifts of the NH2 protons of 9-MeA in DMSO-d6 or DMF-d7 permit a differentiation between the various possibilities (no H bonding, single H bond, 2 H bonds, 1 Pt or 2 Pt coordinated to 9-MeA). As far as intermol. H bonding is concerned, the neutral 9-MeGH ligand in 1b forms a Watson-Crick pair with 1-MeC but a 9-MeGH-9-MeG pair at pH 8. The potential usefulness of the complexes prepd. with regard to the formation of two-dimensional sheet structures and mol. squares built up of purine nucleobase and trans-a2PtII entities is briefly discussed, as are aspects of the stabilization of triplex nucleic acid structures by metal ions.

ACCESSION NUMBER: 1996:222444 CAPLUS
DOCUMENT NUMBER: 124:330618
TITLE: Bis(purine) Complexes of trans-a2PtII: Preparation and X-ray Structures of Bis(9-methyladenine) and Mixed 9-Methyladenine, 9-Methylguanine Complexes and Chemistry Relevant to Metal-Modified Nucleobase Triples and Quartets
AUTHOR(S): Schreiber, Andre; Lueth, Marc S.; Erxleben, Andrea; Fusch, Edda C.; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, D-44221, Germany
SOURCE: Journal of the American Chemical Society (1996), 118(17), 4124-32
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

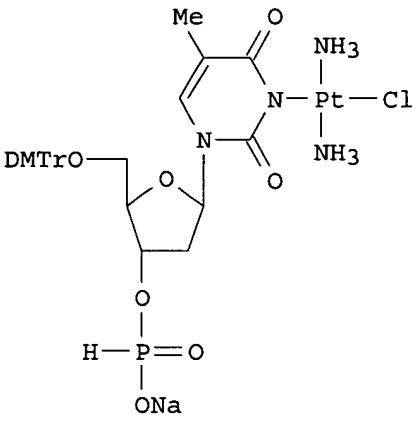
IT **149951-64-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of platinum amine purine base complex)

RN 149951-64-4 CAPLUS
CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



L7 ANSWER 27 OF 87 CAPLUS COPYRIGHT 2003 ACS

GI



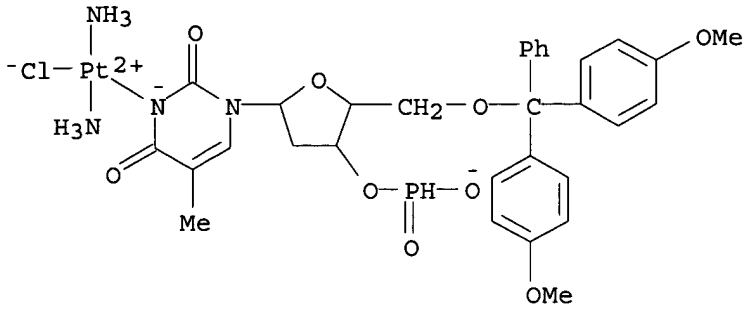
I

AB Platinated nucleoside phosphonate I.bul.KCl was prepd. as synthon for Merrifield synthesis of platinated oligodeoxyribonucleotides.

ACCESSION NUMBER: 1996:211371 CAPLUS
DOCUMENT NUMBER: 125:11330
TITLE: Automated solid phase synthesis of platinated oligodeoxyribonucleotides via nucleoside phosphonates
AUTHOR(S): Schliepe, Juergen; Berghoff, Ulrich; Lippert, Bernd; Cech, Dieter
CORPORATE SOURCE: Fachbereich Chemie, Humboldt-Universitaet, Berlin, D-10099, Germany
SOURCE: Angewandte Chemie, International Edition in English (1996), 35(6), 646-8
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **176907-12-3P 176907-13-4P 176907-14-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Merrifield synthesis of platinated oligodeoxyribonucleotides via nucleoside phosphonates)

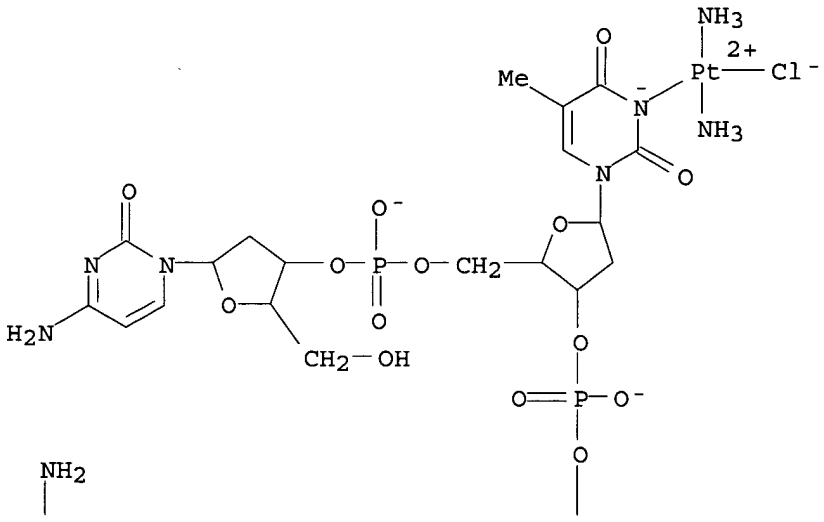
RN 176907-12-3 CAPLUS
CN Platinate(1-), diammine[[5'-O-[bis(4-methoxyphenyl)phenylmethyl]thymidine-.kappa.N3] 3'-(phosphinato)(2-)]chloro-, sodium, (SP-4-2)- (9CI) (CA INDEX NAME)



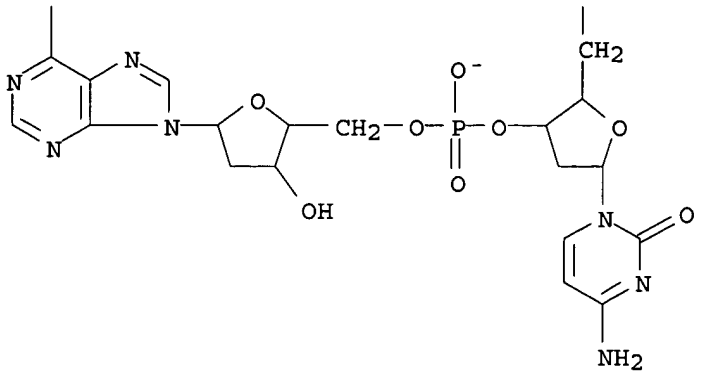
● Na^+

RN 176907-13-4 CAPLUS
CN Platinate(3-), diamminechloro[2'-deoxycytidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2'-deoxyadenosinato(4-)]-, trihydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



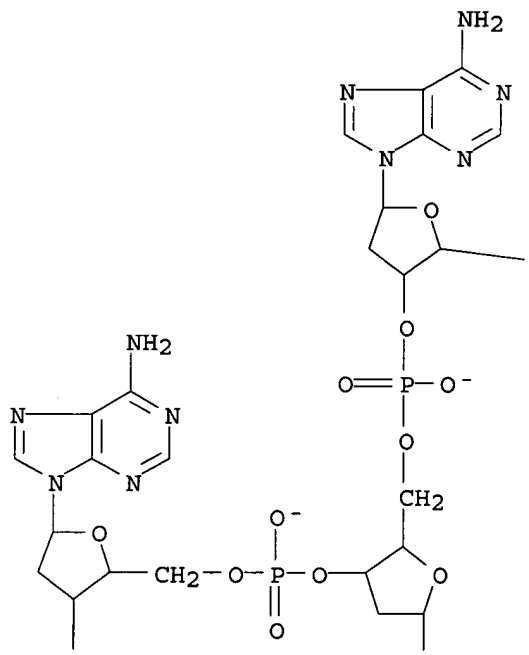
PAGE 2-A



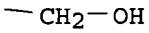
●3 H^+

RN 176907-14-5 CAPLUS
CN Platinate(11-), diamminechloro[deoxyribonucleato(12-) d(A-T-A-G-T-A-T-A-C-A-G-A)]-, undecahydrogen, (SP-4-2)- (9CI) (CA INDEX NAME)

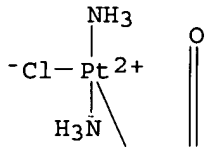
PAGE 1-B



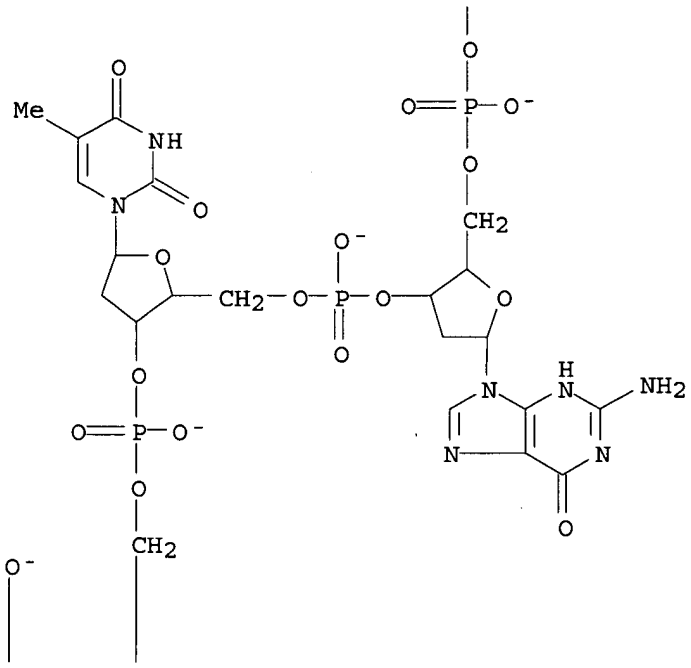
PAGE 1-C

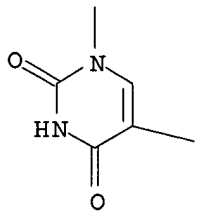


PAGE 2-A



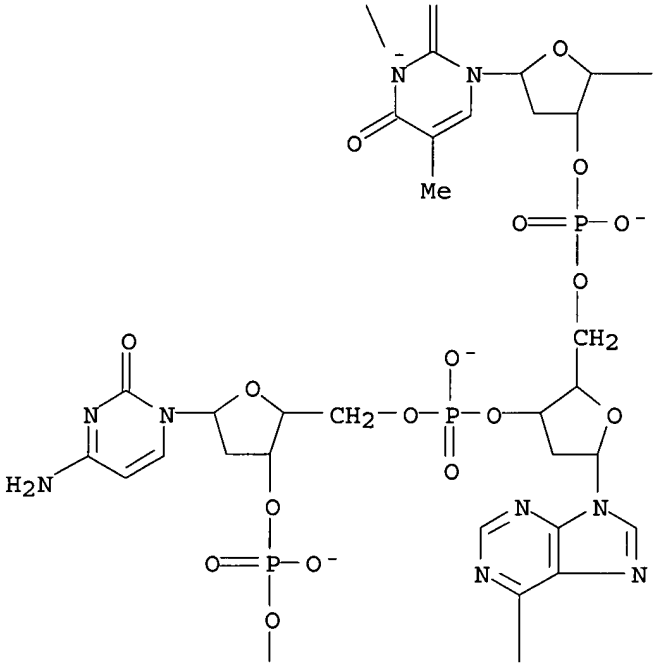
PAGE 2-B



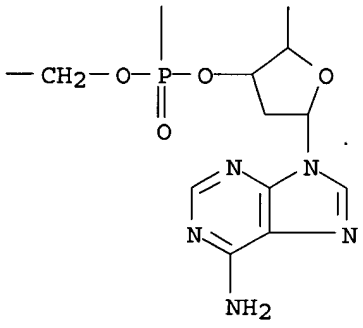


PAGE 2-C

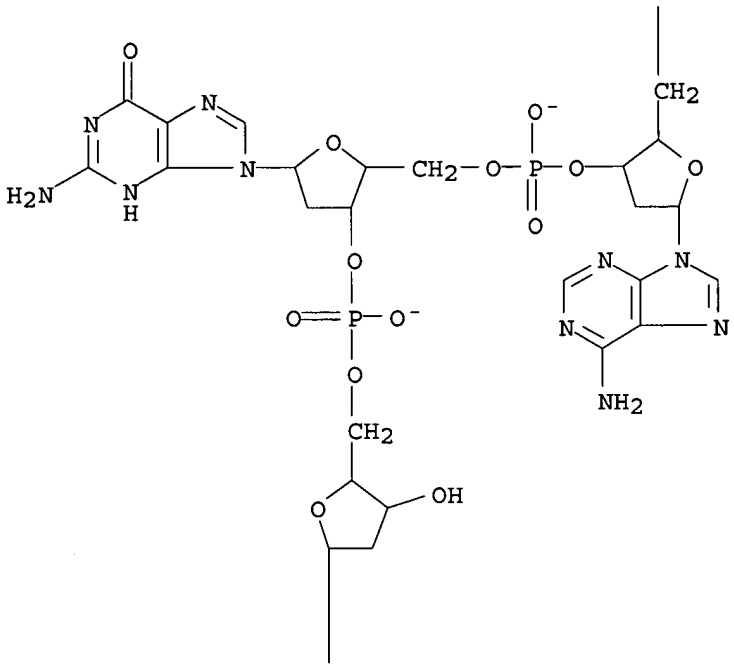
PAGE 3-A



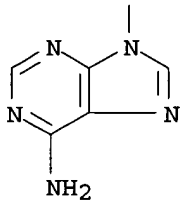
PAGE 3-B



PAGE 4-A



PAGE 5-A



●11 H^+

L7 ANSWER 28 OF 87 CAPLUS COPYRIGHT 2003 ACS

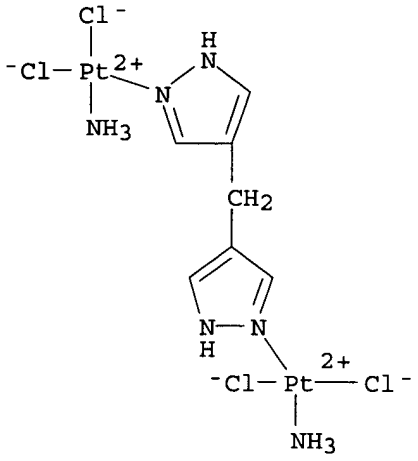
AB Monobridged-dinuclear Pt(II) complexes, where the bridging ligand is 4,4'-dipyrazolylmethane (dpzm), were prepd. for use as potential anticancer agents. The complexes synthesized include [{cis-PtCl2(NH3)}2(.mu.-dpzm)], [{trans-PtCl2(Me2SO)}2(.mu.-dpzm)] and [{cis-PtCl2(Me2SO)}2(.mu.-dpzm)]. The characterization of these complexes is based on microanal., IR and 1H NMR data.

ACCESSION NUMBER: 1996:104236 CAPLUS
DOCUMENT NUMBER: 124:248674
TITLE: The synthesis and characterization of dinuclear platinum complexes bridged by the 4,4'-dipyrazolylmethane ligand
AUTHOR(S): Broomhead, John A.; Lynch, Mark J.
CORPORATE SOURCE: Department of Chemistry, Australian National University, Canberra, ACT, 0200, Australia
SOURCE: Inorganica Chimica Acta (1995), 240(1-2), 13-17
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **174585-20-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and IR spectra and anticancer activity)

RN 174585-20-7 CAPLUS

CN Platinum, diamminetetrachloro[.mu.-[4,4'-methylenebis[1H-pyrazole]-N2:N2']]di-, stereoisomer (9CI) (CA INDEX NAME)

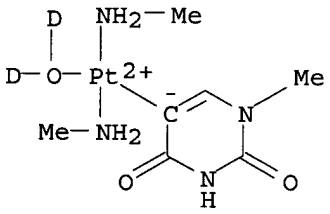


L7 ANSWER 29 OF 87 CAPLUS COPYRIGHT 2003 ACS

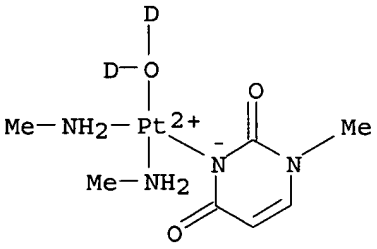
AB 1,3-Dimethyluracil (1,3-DimeU) reacts with trans-[(CH3NH2)2Pt(H2O)2]2+ to give trans-[(CH3NH2)2Pt(1,3-DimeU-C5)(H2O)]X (X = NO3-, 1a, ClO4-, 1b) and subsequently with NaCl to give trans-(CH3NH2)2Pt(1,3-DimeU-C5)Cl (2) or with NH3 to yield trans-[(CH3NH2)2Pt(1,3-DimeU-C5)(NH3)]ClO4 (3). In a similar way, (dien)PtII forms [dienPt(1,3-DimeU-C5)]+ (4). Reactions giving 1 and 4 are slow, taking days. In contrast, Hg(CH3COO)2 reacts fast with 1,3-DimeU to give (1,3-DimeU-C5)Hg(CH3COO) (5). Both 1-methyluracil (1-MeUH) and uridine (urdH) react with (dien)PtII initially at N(3) and subsequently with either (dien)PtII or Hg(CH3COO)2 also at C(5) to give the diplatinated species or a mixed PtHg complex. C(5) binding of either PtII or HgII is evident from coupling of uracil-H(6) with either 195Pt or 199Hg nuclei and 3J values of 47-74 Hz (for Pt compds.) and 185-197 Hz (for Hg compds.). J values of Pt compds. are influenced both by the ligands trans to the uracil C(5) position and by the no. of metal entities bound to a uracil ring. Both 2 and 5 were x-ray structurally characterized. 2: Monoclinic system, space group P21/c, a 15.736(6), b 11.481(6), c 25.655(10) .ANG., .beta. 145.55(3).degree., Z = 4. 5: Monoclinic system, space group P21/c, a 4.905(2), b 18.451(6), c 11.801(5) .ANG., .beta. 94.47(3).degree., Z = 4.

ACCESSION NUMBER: 1996:369 CAPLUS
DOCUMENT NUMBER: 124:176464
TITLE: Uracil C(5) Position as a Metal Binding Site: Solution and x-ray Crystal Structure Studies of PtII and HgII Compounds
AUTHOR(S): Hoepp, Markus; Erxleben, Andrea; Rombeck, Ingo; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, 44221, Germany
SOURCE: Inorganic Chemistry (1996), 35(2), 397-403
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

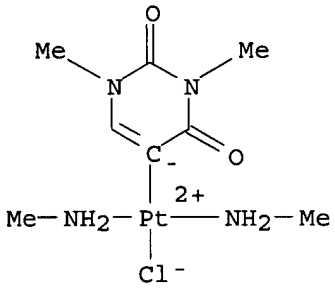
IT **173776-52-8P**
RL: BYP (Byproduct); PREP (Preparation)
(formation from platinum amine uracilato and platinum amine aqua complexes)
RN 173776-52-8 CAPLUS
CN Platinum(1+), aqua-d2-bis(methanamine)(1,2,3,4-tetrahydro-1-methyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **173776-51-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation from platinum amine uracilato and platinum amine aqua complexes)
RN 173776-51-7 CAPLUS
CN Platinum(1+), aqua-d2-bis(methanamine)(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



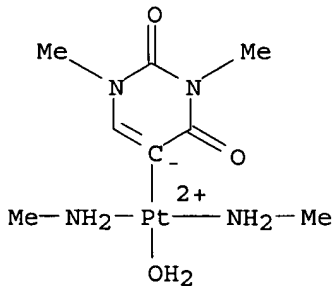
IT **173776-38-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)
RN 173776-38-0 CAPLUS
CN Platinum, chlorobis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **173776-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with aq. ammonia)
RN 173776-53-9 CAPLUS
CN Platinum(1+), aquabis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)-, perchlorate (9CI) (CA INDEX NAME)

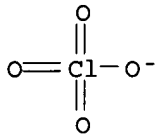
CM 1

CRN 173776-36-8
CMF C8 H19 N4 O3 Pt
CCI CCS



CM 2

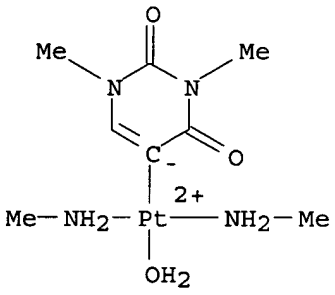
CRN 14797-73-0
CMF Cl O4



IT **173776-37-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with chloride)
RN 173776-37-9 CAPLUS
CN Platinum(1+), aquabis(methanamine)(1,2,3,4-tetrahydro-1,3-dimethyl-2,4-dioxo-5-pyrimidinyl)-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

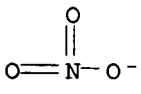
CM 1

CRN 173776-36-8
CMF C8 H19 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



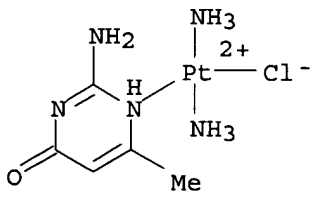
ANSWER 30 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The growth-inhibiting effect on the roots of maize and cucumber shoots was studied. We tested 53 triamine complexes of platinum (cis*- and trans*-[Pt(NH3)2*LCl]Cl, cis*- and trans*-[PtHx2* Lcl]Cl and [PtenLCl]Cl, where Hx is hydroxylamine, en is ethylenediamine, and L are various heterocycles, which either have biol. activity and occur in the cells or have no biol. activity and are foreign to the cells). The cis*-[Pt(NH3)2*LCl]Cl and [PtenLCl]Cl complexes showed cytostatic properties, and the latter were effective at higher concns. Small changes in the compn. of ligand L led to marked changes in the biol. activity of the complexes. In order to characterize the effect of the complexes, we first detd. the time of development of the lateral root from its initial appearance to its divergence from the main root (Tlat). The complexes with cytostatic properties markedly inhibited root branching and increased Tlat. The other complexes had virtually no effect on Tlat and reduced the zone of lateral roots only at the expense of inhibition of the main root growth. The complexes with cytostatic properties markedly inhibited the main root growth. The complexes with cytostatic properties markedly inhibited the main root growth with time. Parallel studies conducted in the Oncol. Research Center, Russian Academy of Medical Sciences have shown that the complexes with cytostatic properties display distinct antitumor activity.

ACCESSION NUMBER: 1995:768308 CAPLUS
DOCUMENT NUMBER: 123:275180
TITLE: Biological activity of platinum(II) complexes of the triamine type as a function of their composition and structure
AUTHOR(S): Ivanov, V. B.; Bystrova, E. I.; Larina, L. P.; Yakovlev, K. I.; Stetsenko, A. I.; Ivanova, L. I.; Imsyrova, A. F.; Iozen, L. I.; Tikhonova, L. S.
CORPORATE SOURCE: Kurnakov Inst. of General and Inorganic Chemistry, Moscow, 117907, Russia
SOURCE: Izvestiya Akademii Nauk, Seriya Biologicheskaya (1995), (3), 281-90
CODEN: IRABEC
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

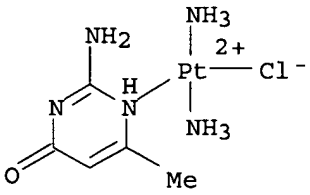
IT **169231-47-4 169275-48-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(biol. activity of platinum(II) complexes of the triamine type as function of their compn. and structure)

RN 169231-47-4 CAPLUS
CN Platinum(1+), (2-amino-6-methyl-4(1H)-pyrimidinone-N1)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



⊙ Cl -

RN 169275-48-3 CAPLUS
CN Platinum(1+), (2-amino-6-methyl-4(1H)-pyrimidinone-N1)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



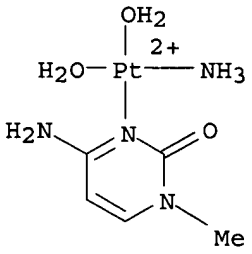
L7 ANSWER 31 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Trans-Pt(NH3)(1-MeC-N3)I2 (4) with 1-MeC (1-methylcytosine) bound to Pt via N(3), obtained from cis-[Pt(NH3)2(1-MeC-N3)Cl]Cl, gives trans-[Pt(NH3)(1-MeC-N3)(H2O)2]2+ when treated with 2 equiv of AgNO3. This diaqua species rapidly dimerizes in soln. to give [Pt2(NH3)2(1-MeC--N3,N4)2(H2O)2]2+ (5), a compd. contg. bridging 1-methylcytosinato ligands in a head-tail arrangement, as judged from 1H NMR spectroscopy. Also an intensely purple, paramagnetic species 5' forms, which is yet another representative of the class of Pt pyrimidine blues. If dimerization to give 5 is carried out in the presence of the amino acid glycine, spontaneous oxidn. to a yellow diplatinum(III) complex [Pt2(NH3)2(1-MeC--N3,N4)2(gly-N,O)2](NO3)2.cntdot.3H2O (6) takes place. The compd. was isolated and characterized by NMR spectroscopy (1H, 195Pt) and x-ray crystallog.: triclinic system, space group P.hivin.1, a 12.438(4), b 12.820(4), c 10.275(2) .ANG., .alpha. 98.21(3), .beta. 112.84(2), .gamma. 62.24(2).degree., Z = 2. In 6, the two methylcytosinato rings are oriented head-tail, and glycinate anions chelate Pt atoms via NH2 (axial) and COO- (equatorial). The Pt-Pt bond length is 2.527(1) .ANG.. When L-alanine is applied instead of glycine, a complex analogous to 6 is formed which occurs in soln. in two diastereomeric forms, however, as evident from 1H NMR spectroscopy. From 5, an oligomerization process leading to Pt cytosine blue is proposed, according to which O(2) of 1-MeC- is involved in bridging dinuclear entities or dinuclear and mononuclear entities. The proposed oligomerization principle differs markedly from that obsd. in tetranuclear (Pt2.25+)4 complexes contg. cyclic amidate ligands.

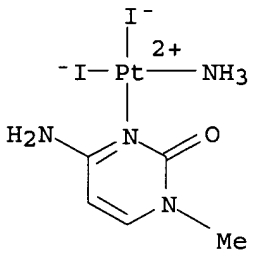
ACCESSION NUMBER: 1995:380922 CAPLUS
DOCUMENT NUMBER: 122:150172
TITLE: Dimerization of trans-[Pt(NH3)(1-MeC-N3)(H2O)2]2+ and Oxidation to a Diplatinum(III) Species in the Presence of Glycine. Relevance for Platinum Cytosine Blue
AUTHOR(S): Wienkoetter, Thomas; Sabat, Michal; Fusch, Gerd; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, D-44221, Germany
SOURCE: Inorganic Chemistry (1995), 34(5), 1022-9
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **161269-46-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(formation and dimerization with/without oxidn. in presence of amino acids)

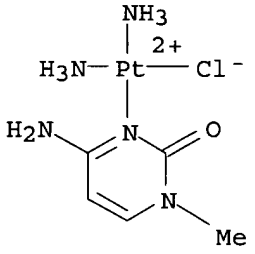
RN 161269-46-1 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)amminediaqua-, (SP-4-1)- (9CI) (CA INDEX NAME)



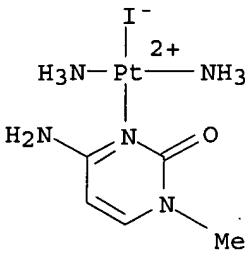
IT **161269-39-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and aquation using silver nitrate)
RN 161269-39-2 CAPLUS
CN Platinum, (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)amminediiodo-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT **75659-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with potassium iodide)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **161269-38-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 161269-38-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineiodo-, iodide, (SP-4-3)- (9CI) (CA INDEX NAME)



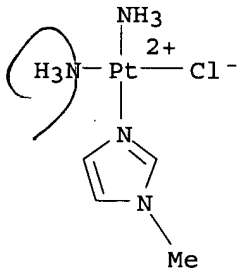
L7 ANSWER 32 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Ternary complexes of Pt(II) with the nucleotides 5'-GMP, 3'-GMP and 5'-dGMP (GMP = guanosine monophosphate), and with the amino acids N.alpha.-BOC-L-histidine, N.alpha.-BOC-L-methionine and 1-methylimidazole (1-MeIm) were studied as models for Pt mediated DNA-protein crosslinks. The triamine complexes [PtAm2(L)Cl]+ (where Am2 = cis- or trans-(NH3)2 or ethylenediamine and L = 1-MeIm or N.alpha.-BOC-L-his-N3) react readily with the mononucleotides 5'-GMP, 3'-GMP and 5'-dGMP to form the ternary crosslinked complexes PtAm2(L)(nucleotide). The 5'-nucleotides react faster than their 3' counterparts towards either triamine complex. Kinetic studies by 1H NMR show that cis-[PtAm2(1-MeIm-N3)Cl]+ reacts with 5'-GMP faster than the trans isomer (second order rate consts. k2 = 0.756 and 0.358 M-1 s-1, resp.) and that the ethylenediamine complex is faster than both (k2 = 1.09 M-1 s-1).

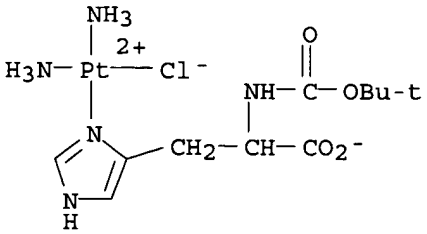
ACCESSION NUMBER: 1994:524676 CAPLUS
DOCUMENT NUMBER: 121:124676
TITLE: Ternary Pt(II)-amino acid-nucleotide complexes: kinetics of formation
AUTHOR(S): Gibson, Dan; Arvanitis, Georgia M.; Berman, Helen M.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, School of Pharmacy, The Hebrew University of Jerusalem, Jerusalem, Israel
SOURCE: Inorganica Chimica Acta (1994), 218(1-2), 11-19
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **157080-02-9P 157207-98-2P 157242-49-4P**
RL: PREP (Preparation)
(prep. and ternary tetraamine complexation of)

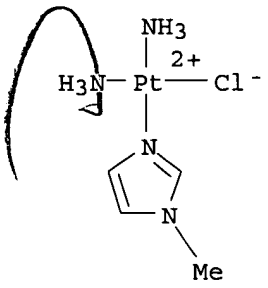
RN 157080-02-9 CAPLUS
CN Platinum(1+), diamminechloro(1-methyl-1H-imidazole-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 157207-98-2 CAPLUS
CN Platinum, diamminechloro[N-[(1,1-dimethylethoxy)carbonyl]-L-histidinato-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 157242-49-4 CAPLUS
CN Platinum(1+), diamminechloro(1-methyl-1H-imidazole-N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



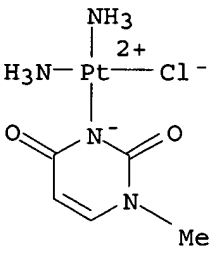
L7 ANSWER 33 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The substitution behavior of cis-Pt(NH3)2(1-MeU)2, cis-Pt(NH3)2(1-MeU)Cl and cis-[Pt(NH3)2(1-MeU)H2O]+ (1-MeU = 1-methyluracil anion, C5H5N2O2) was studied in detail as a function of entering nucleophile concn., pH, temp., and pressure. The reactivity of these species is controlled by the lability of the aqua complex. Protonation of the exocyclic O(4) atom of the 1-methyluracil ligand is essential in order to increase the lability of the bis(methyluracilato) complex. Solvolysis is the rate-detg. step for substitution reactions of the latter complex, for which k = (2.40 .+-. 0.06) .times. 10-5 s-1 at 60.degree. and pH = 3, .DELTA.H.thermod. = 79 .+-. 1 kJ mol-1, .DELTA.S.thermod. = -98 .+-. 11 JK-1 mol-1, and .DELTA.V.thermod. = -5.6 .+-. 0.6 cm3 mol-1. All the reported rate and activation parameters support the operation of an associative substitution mechanism. The results are discussed in ref. to data reported in the literature for related systems.

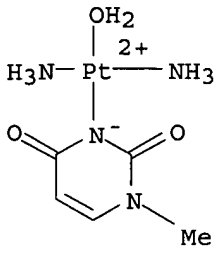
ACCESSION NUMBER: 1994:466680 CAPLUS
DOCUMENT NUMBER: 121:66680
TITLE: Kinetics and Mechanism of the Substitution Reactions of cis-Diamminebis(1-methyluracilato)platinum(II) in Aqueous Solution
AUTHOR(S): Schmuelling, Michael; Lippert, Bernhard; van Eldik, Rudi
CORPORATE SOURCE: Institut fuer Anorganische Chemie, Universitaet Witten/Herdecke, Witten, 58448, Germany
SOURCE: Inorganic Chemistry (1994), 33(15), 3276-80
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-78-2 85715-79-3**
RL: PRP (Properties)
(substitution reaction kinetics and mechanism of)

RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 85715-79-3 CAPLUS
CN Platinum(1+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



ANSWER 34 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. and crystal structure of cis,cis-[(NH3)2Pt(1-MeT)2(OH)(H2O)]AuCl4.H2O (I; 1-MeTH = 1-methylthymine) is reported. I contains both heterocyclic bases bound to Pt via the N3 positions, the 2 nucleobase ligands being in a head-to-head orientation. I crystallizes as triclinic, space group P.hivin.1, a 8.435(4), b 11.884(3), c 12.869(7) .ANG., .alpha. 97.28(3), .beta. 91.66(5), .gamma. 110.66(5).degree., Z = 2, R = 0.056, Rw = 0.065.

ACCESSION NUMBER: 1994:152111 CAPLUS
DOCUMENT NUMBER: 120:152111
TITLE: Formation and x-ray crystal structure analysis of a platinum(IV) complex of 1-methylthymine, obtained through gold(III) treatment of a Pt(II) complex
AUTHOR(S): Renn, Oliver; Lippert, Bernhard; Albinati, Alberto; Lianza, Francesca
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Dortmund, Dortmund, D-44221, Germany
SOURCE: Inorganica Chimica Acta (1993), 211(2), 177-82
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **151591-41-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and IR and XPS spectra of)

RN 151591-41-2 CAPLUS

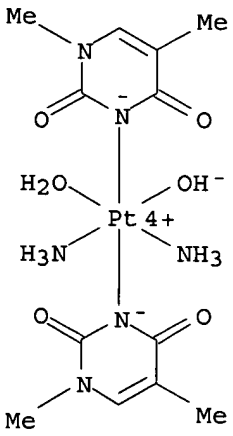
CN Platinum(1+), diammineaquabis(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-N3)hydroxy-, (OC-6-24)-, (SP-4-1)-tetrachloroaurate(1-), monohydrate (9CI) (CA INDEX NAME)

CM 1

CRN 151591-40-1
CMF C12 H23 N6 O6 Pt . Au Cl4

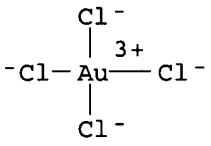
CM 2

CRN 151591-39-8
CMF C12 H23 N6 O6 Pt
CCI CCS



CM 3

CRN 14337-12-3
CMF Au Cl4
CCI CCS



L7 ANSWER 35 OF 87 CAPLUS COPYRIGHT 2003 ACS

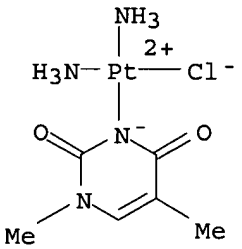
AB Linking 3 nucleobases by 2 metal ions M of linear coordination geometry leads to metal-modified base triples. With M = trans-(amine)2PtII, the bases are forced into an essentially coplanar fashion with interbase H bonding maintained in many cases. The model nucleobase triples described here are {[trans-(amine)2PtL]2(9-MeA)}n+ with 2 nucleobases L (9-methyladenine, 9-ethylguanine, 1-methylthymine, 1-methylcytosine, cytosine) bound via Pt to N1 and N7 of 9-methyladenine (9-MeA). The x-ray structure of a precursor, {[trans-(MeNH2)2PtCl]2(9-MeA)}(ClO4)2, is briefly described. The generation of metalated, cyclic nucleobase quartets and their expected structures are discussed and ways towards larger macrocyclic metal compds. are pointed out.

ACCESSION NUMBER: 1994:123417 CAPLUS
DOCUMENT NUMBER: 120:123417
TITLE: On metal-modified nucleobase triples and quartets
AUTHOR(S): Schreiber, Andre; Hillgeris, Edda C.; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-44221, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1993), 48(11), 1603-12
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149951-64-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silver nitrate followed by platinum ammine methyladenine methylthymine complex)

RN 149951-64-4 CAPLUS

CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



ANSWER 36 OF 87 CAPLUS COPYRIGHT 2003 ACS

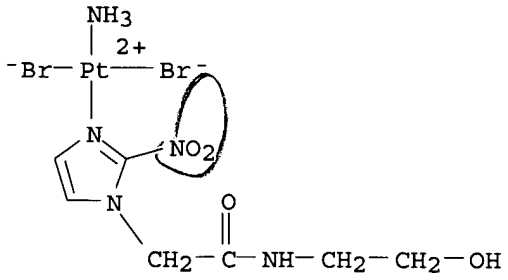
AB Cis-[PtBr2L(NH3)] (L = N-(2-hydroxyethyl)-2-nitroimidazole-1-acetamide (etanidazole)) was prepd. and crystd. in orthorhombic, space group Pnca, Z = 8, R = 0.062. Pt has a square-planar coordination. The Pt-Br bond trans to the nitroimidazole ligand is slightly shorter [2.375 (3) .ANG.] than the Pt-Br bond trans to NH3 [2.397 (3) .ANG.]. The dihedral angle between the Pt coordination plane and the imidazole ring is 69.1.degree., while the nitro group makes an angle of 32.degree. with the imidazole ring plane. The structure is stabilized by the hydrogen bonding of the NH3 ligands and the hydroxyl groups. The crystal structure was also detd. for trans-[PdCl2L'2] (L' = 2-methyl-5-nitroimidazole-1-ethanol (metronidazole)) monoclinic, space group P21/c, Z = 2, R = 0.027. The bond distances Pd-Cl = 2.297 (1) and Pt-N = 2.007 (2) .ANG.. The dihedral angle between the Pd coordination plane and the imidazole ring is 88.6 (1).degree., while the nitro groups make an angle of 3.9(3).degree. with the imidazole plane. The structure is stabilized by hydrogen bonding between the hydroxyl groups and the chloro ligands.

ACCESSION NUMBER: 1994:123362 CAPLUS
DOCUMENT NUMBER: 120:123362
TITLE: Structures of the nitroimidazole platinum group metal complexes: cis-amminedibromo[1-({[(2-hydroxyethyl)amino]carbonyl}methyl)-2-nitroimidazole]platinum(II) and trans-dichlorobis(1-hydroxyethyl-2-methyl-5-nitroimidazole)palladium(II)
AUTHOR(S): Rochon, Fernande D.; Melanson, Robert; Farrell, Nicholas
CORPORATE SOURCE: Dep. Chem., Univ. Quebec, Montreal, QC, H3C 3P8, Can.
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1993), C49(10), 1703-6
CODEN: ACSCEE; ISSN: 0108-2701
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **152837-74-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

RN 152837-74-6 CAPLUS

CN Platinum, amminedibromo[N-(2-hydroxyethyl)-2-nitro-1H-imidazole-1-acetamide-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



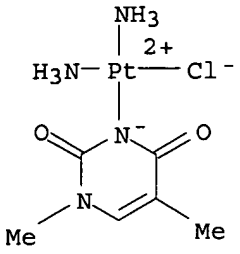
L7 ANSWER 37 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Replacement of a weakly acidic N-H proton of a H bond between 2 nucleobases (neutral or hemiprotonated) by a metal species of suitable geometry generates metal-modified nucleobase pairs. Depending upon the combination of bases and/or resp. donor sites involved in metal binding, these adducts can be divided in metal analogs of (i) homopyrimidine and homopurine pairs, (ii) Watson-Crick pairs, (iii) Hoogsteen pairs, (i.v.) pairs between noncomplementary bases, and (v) nonnucleobase, nucleobase pairs. Representative examples of (ii)-(v) were prepd. and are reported. In 3 cases, (ii), (iii), and (v), x-ray crystallog. was used to det. structural details. Trans-[(MeNH2)2Pt(1-MeT-N3)(9-MeA-N1)]ClO4.3.25H2O (4') crystallizes in the triclinic space group P1 with Z = 2. Trans-[(NH3)2Pt(1-MeT-N3)(9-MeA-N7)]ClO4.2.5H2O (5) crystallizes in the same space group P1 with Z = 4. Trans-[(NH3)2Pt(2-NH2-py)(9-MeGH-N7)](NO3)2 (10) (2-NH2-py = 2-aminopyridine) crystallizes in the monoclinic space group P21/c with Z = 4. In 4', the 2 complementary bases 1-methylthymine (deprotonated at N3) and 9-methyladenine are arranged in a Watson-Crick fashion, while in 5 they adopt a Hoogsteen arrangement. In both cases a (partial) disorder of the 1-MeT ligand cannot be excluded from x-ray data. With 5, variable temp. 1H NMR spectroscopy in DMF-d7 was applied to demonstrate the existence of rotamers (Hoogsteen and reversed Hoogsteen arrangement of the nucleobases) in soln. Common structural features of 4', 5, and 10 are an approx. coplanar arrangement of the 2 heterocyclic ligands, a marked nonlinearity of the base-Pt-base' angle (deviation as much as 173.4(2).degree. in 4'), and H bonding between the 2 bases. This H bonding occurs between exocyclic groups of the bases intramolecularly in 5 and 10 and via a H2O mol. in 4'. Structural changes of the adenine, thymine base pair upon metal modifications are discussed in detail, extended to other metals (AgI, HgII), and generalized to other possible metal coordination geometries. The formation of metal-modified base pairs, with regard to DNA crosslinking and related topics, is discussed.

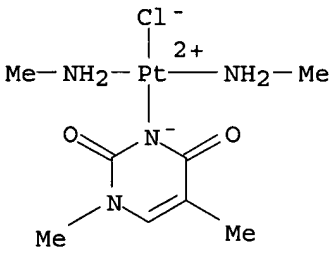
ACCESSION NUMBER: 1993:572860 CAPLUS
DOCUMENT NUMBER: 119:172860
TITLE: Metal-modified nucleobase pairs: mixed adenine, thymine complexes of trans-a2platinum(II) (a = ammonia, methylamine) with Watson-Crick and Hoogsteen orientations of the bases
AUTHOR(S): Krizanovic, Olga; Sabat, Michal; Beyerle-Pfnuer, Rut; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, 4600, Germany
SOURCE: Journal of the American Chemical Society (1993), 115(13), 5538-48
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **149951-64-4P 150120-54-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with silver perchlorate followed by methyladenine)

RN 149951-64-4 CAPLUS
CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



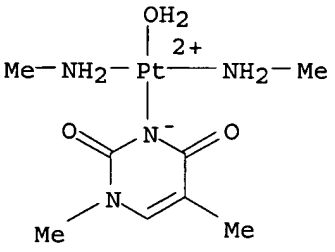
RN 150120-54-0 CAPLUS
CN Platinum, chloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)bis(methanamine)-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **150120-79-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylguanine)
RN 150120-79-9 CAPLUS
CN Platinum(1+), aqua(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-N3)bis(methanamine)-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

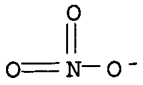
CM 1

CRN 150120-78-8
CMF C8 H19 N4 O3 Pt
CCI CCS



CM 2

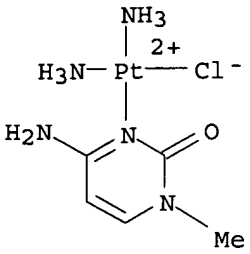
CRN 14797-55-8
CMF N O3



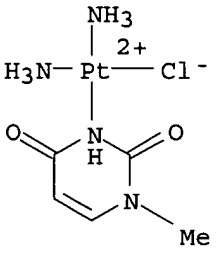
L7 ANSWER 38 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Reactions of L-histidine, N-acetyl-L-histidine, and glycyl-L-histidine with monofunctional species [(dien)M(H2O)]2+ (M = Pt, Pd; dien = diethylenetriamine), [(trpy)M(H2O)]2+ (trpy = terpyridine), cis-[(NH3)2Pt(1-MeU)(H2O)]+ (1-MeUH = 1-methyluracil), cis-[(NH3)2Pt(1-MeC)(H2O)]2+ (1-MeC = 1-methylcytosine), and trans-[(NH2Me)2Pt(1-MeC)(H2O)]2+) were studied by applying primarily 1H NMR and, in some cases, 195Pt NMR spectroscopy. Depending on reaction conditions (pH; M:ligand ratio), different products are formed which, in the case of N-acetylhistidine and (dien)PtII, for example, include monodentate coordination through N1 of imidazole, N3 of imidazole, and O of carboxylate or bidentate bridging via N1,O, and N3,O, and N1,N3. With L-histidine and (dien)PtII, formation of an isomer with coordination through the amino group is obsd., which takes place by a migration process from the initially favored O site. In the case of the ternary nucleobase/N-acetylhistidine complexes of PtII, N1 and N3 linkage isomers were sepd. using HPLC and isolated in a few cases and their acid/base equil. detd. The formation of N1 and N3 linkage isomers, which correspond to the metalated forms fo the resp. tautomers, is the outstanding feature of this study. The differentiation of tautomers of the Pt compds. in many cases is straightforward in spectra recorded at low magnetic field (80-100 MHz) when 195Pt-1H (imidazole) couplings are observable. The methine resonances of the 2 isomers differ, with those of the N3 isomers downfield relative to those of the N1 isomer. From published data on the tautomer distribution and the measured distribution of (dien)PdII over the 2 imidazole sites, probably PdII complex formation with N1 is slightly favored over N3 in the case of N-acetylhistidine, but substantially more so in the case of L-histidine. As for (dien)PtII, the distribution of imidazole-bound isomers reflects primarily kinetic rather than thermodn. factors.

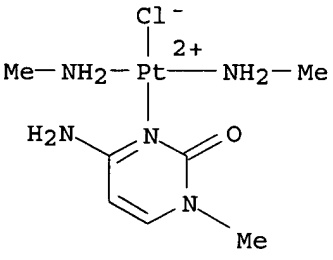
ACCESSION NUMBER: 1992:583668 CAPLUS
DOCUMENT NUMBER: 117:183668
TITLE: Linkage isomerism in square-planar complexes of platinum and palladium with histidine and derivatives
AUTHOR(S): Appleton, Trevor G.; Pesch, Ferdinand J.; Wienken, Markus; Menzer, Stephan; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-4600, Germany
SOURCE: Inorganic Chemistry (1992), 31(21), 4410-19
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **75659-46-0 89061-11-0 128636-28-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with silver nitrate followed by acetylhistidine)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 89061-11-0 CAPLUS
CN Platinum(1+), diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedione-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 128636-28-2 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)chlorobis(methanamine)-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



ANSWER 39 OF 87 CAPLUS COPYRIGHT 2003 ACS

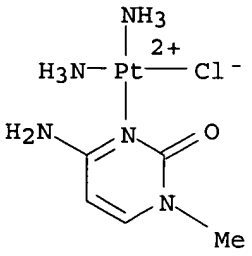
AB The reactions of trans-[(NH3)2Pt(nucl)Cl]Z (Z = Cl-, nucl = 9-methylguanine; Z = NO3-, nucl = 1-methylcytosine) with AgNO3 followed by the amino acids (Haa) glycine, L-alanine, 2-L-aminobutyric acid, L-valine and L-norvaline, in aq. solns., produced 7 trans-[(NH3)2Pt(nucl)(aa)]NO3.mH2O (m = 0, 2). Protonation of these by HNO3 or HClO4 gave 3 trans-[(NH3)2Pt(nucl)(Haa)]Z2.nH2O (Z = NO3-, ClO4-; n = 0, 1). The complexes were characterized in the solid state with elemental anal., cond. measurements, IR and 1H NMR spectra. Both nucleobases retain their N3 and N7 coordinations in the ternary systems. Weak hydrophobic ligand-ligand interactions were obsd. in soln. with 1H NMR in the present system, weaker even than in the corresponding cis system.

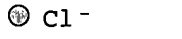
ACCESSION NUMBER: 1992:562811 CAPLUS
DOCUMENT NUMBER: 117:162811
TITLE: Ternary complexes of trans-diamminedichloroplatinum with amino acids and nucleobases
AUTHOR(S): Aletras, V.; Hadjiliadis, N.; Lippert, B.
CORPORATE SOURCE: Dep. Chem., Univ. Ioannina, Ioannina, 45-110, Greece
SOURCE: Polyhedron (1992), 11(11), 1359-67
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **98920-59-3**, trans-Diamminechloro(1-methylcytosine)platinum(1+) chloride
RL: PRP (Properties)
(IR and NMR spectra of)

RN 98920-59-3 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)





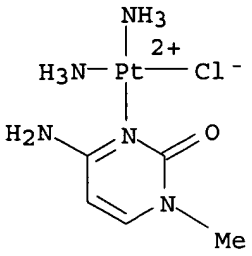
IT **142904-22-1P**, trans-Diamminechloro(1-methylcytosine)platinum(1+) nitrate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with silver nitrate followed by amino acids)

RN 142904-22-1 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, (SP-4-2)-, nitrate (9CI) (CA INDEX NAME)

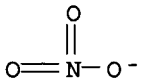
CM 1

CRN 142904-21-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



L7 ANSWER 40 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. and characterization of a series of mono-, di-, and trinuclear Pt(II) complexes of 9-methylguanine (9-MeGH) are reported. The compds. contain the guanine heterocycle monoplatinated at N1 and/or diplatinated at N1 and N7. The route to these compds. involves a primary fixation of a (dien)Pt(II) (dien = diethylenetriamine) entity to the N7 position, fixation of a 2nd Pt(II) at N1, and subsequent removal of the N7-bound Pt(II) by CN-. The crystal structure via x-ray diffraction of a representative example, (en)Pt(9-MeG-N1)2.cntdot.3H2O is reported, tetragonal, space group I41/a, a 16.003(2), c 32.247(6) .ANG., Z = 16, R = 0.027, Rw = 0.022.

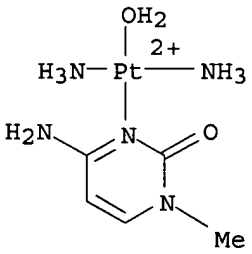
ACCESSION NUMBER: 1992:267860 CAPLUS
DOCUMENT NUMBER: 116:267860
TITLE: Platinum(II) coordination to N1 and N7,N1 of guanine: cis-DDP model cross-links in the interior and simultaneous cross-links at the periphery and the interior of DNA
AUTHOR(S): Frommer, Gudrun; Mutikainen, Ilpo; Pesch, Ferdinand J.; Hillgeris, Edda C.; Preut, Hans; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, 4600, Germany
SOURCE: Inorganic Chemistry (1992), 31(12), 2429-34
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **98874-75-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with platinum diethylenetriamine ethylenediamine methylguanido dinuclear complex)

RN 98874-75-0 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)

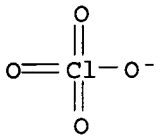
CM 1

CRN 80662-70-0
CMF C5 H15 N5 O2 Pt
CCI CCS

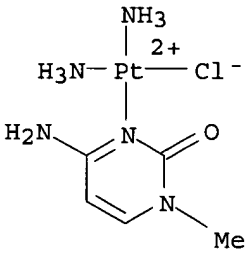


CM 2

CRN 14797-73-0
CMF Cl O4



IT **75659-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silver nitrate followed by platinum nucleotide complexes)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



L7 ANSWER 41 OF 87 CAPLUS COPYRIGHT 2003 ACS

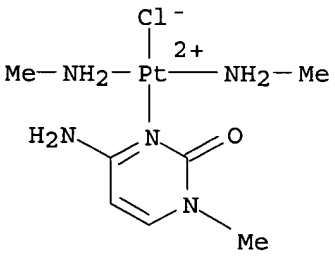
AB The prepn. and x-ray structure of trans-{[(CH3NH2)2Pt(1-MeC)(9-MeGH)]Cl2.(1-MeC)} 0.5 {[(1-MeCH).(1-MeC)]Cl}.4.5H2O, where 1-MeC = 1-methylcytosine and 9-MeGH = 9-methylguanine, is reported. The compd. contains the trans-diamineplatinum(II) entity coordinated to N3 of 1-MeC and to N7 of 9-MeGH with a H bond between the exocyclic NH2(4) of 1-MeC and O(6) of 9-MeGH, thereby representing a metal analog of a Hoogsteen base pair between 1-MeCH+ and 9-MeGH. In addn., 1-MeC is H bonded to the platinated guanine in the known Watson-Crick fashion, and there is also a (1-MeCH+) (1-MeC) base pair with 3 hydrogen bonds between the 2 cytosines. The PtCG.C base triple is a model for a triplex DNA slice in which a pyridine oligonucleotide strand is covalently linked to a GC section of a DNA duplex.

ACCESSION NUMBER: 1992:36391 CAPLUS
DOCUMENT NUMBER: 116:36391
TITLE: Model for a platinated DNA triplex: Watson-Crick and metal-modified Hoogsteen pairing
AUTHOR(S): Dieter-Wurm, Iris; Sabat, Michal; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, 4600, Germany
SOURCE: Journal of the American Chemical Society (1992), 114(1), 357-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **129232-51-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylguanine)

RN 129232-51-5 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)chlorobis(methanamine)-, chloride, monohydrate, (SP-4-2)- (9CI) (CA INDEX NAME)



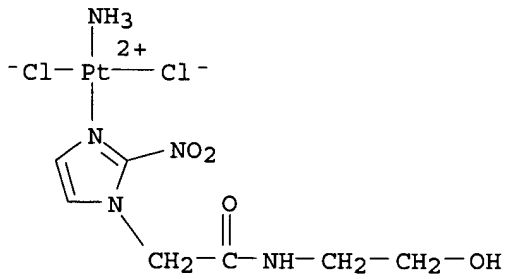
ANSWER 42 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The characterization of [PtCl2(NH3)(NO2Im)] (NO2Im = Etanidazole (L), Misonidazole (L1) and Metronidazole (L2)) is reported. Both cis and trans isomers may be isolated for the L1 and L2 complexes. The crystal structure of cis-[PtCl2(NH3)L] has been detd. by x-ray diffraction. The crystals are orthorhombic, space group Pnab with a 14.867(7), b 9.915(5), c 19.015(9) .ANG., Z = 8, R = 0.062 and Rw = 0.052. Platinum has the expected square-planar coordination. The Pt-Cl bond trans to the nitroimidazole ligand is shorter (2.269(3) .ANG.) than normal. The dihedral angle between the platinum plane and the imidazole ring is 111.degree., while the nitro group makes an angle of 31.degree. with the imidazole ring plane. Electrochem. and 195Pt NMR data are also reported. The relevance of the chem. properties to their biol. properties as radiosensitizers and hypoxic cytotoxins is discussed.

ACCESSION NUMBER: 1991:669138 CAPLUS
DOCUMENT NUMBER: 115:269138
TITLE: Characterization and properties of monoammine nitroimidazole complexes of platinum [PtCl2(NH3)(NO2Im)]. Crystal and molecular structure of cis-amminedichloro(1-{(((2-hydroxyethyl)amino)carbonyl)methyl}-2-nitroimidazole)platinum(II)
AUTHOR(S): Rochon, Fernande D.; Kong, Pi Chang; Melanson, Robert; Skov, Kirsten A.; Farrell, Nicholas
CORPORATE SOURCE: Vermont Reg. Cancer Cent., Univ. Vermont, Burlington, VT, 05405, USA
SOURCE: Inorganic Chemistry (1991), 30(24), 4531-5
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

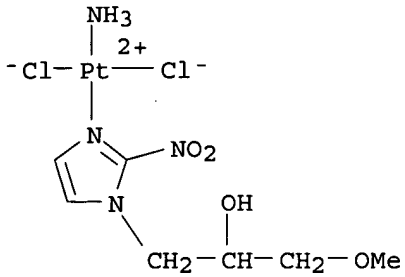
IT **136844-76-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and electrochem. redn. and radiosensitizing and hypoxic cytotoxin properties of)

RN 136844-76-3 CAPLUS
CN Platinum, amminedichloro[N-(2-hydroxyethyl)-2-nitro-1H-imidazole-1-acetamide-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)

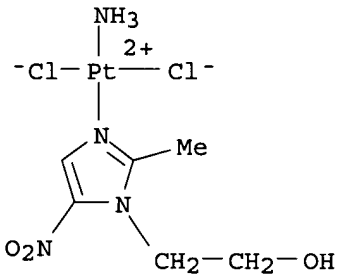


IT **114532-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and electrochem. redn. and radiosensitizing and hypoxic cytotoxin properties of)

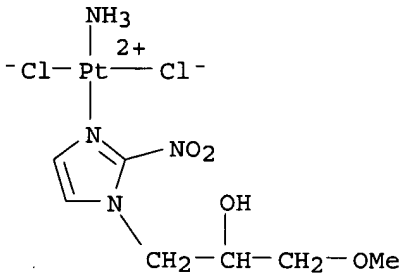
RN 114532-23-9 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-1)- (9CI) (CA INDEX NAME)



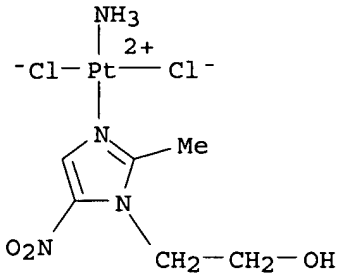
IT **110321-22-7P 112198-62-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and isomerization and electrochem. redn. and radiosensitizing and hypoxic cytotoxin properties of)
RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 112198-62-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **121350-06-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. by isomerization and electrochem. redn. and radiosensitizing and hypoxic cytotoxin properties of)
RN 121350-06-9 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-1)- (9CI) (CA INDEX NAME)



L7 ANSWER 43 OF 87 CAPLUS COPYRIGHT 2003 ACS

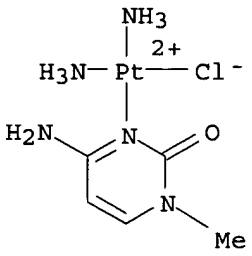
AB cis-Pt(NH3)2LQ (HL = glycine (GlyH), L-alanine, L-2-aminobutyric acid, L-valine and L-norvaline; HQ = 1-methylcytosine (1-MeCH) and 9-methylguanine (9-MeGH)) were prepd. in aq. solns. via two synthetic routes: by reacting the binary complexes, either cis-[(NH3)2PtL](NO3) with HQ (route 1)), or the cis-[(NH3)2PtQCl](NO3) with the amino acids. The amino acids are monodentate (coordination through NH2) and their carboxylate groups are deprotonated. The nucleobases coordinate through N(3) (1-MeC) and N(7) (9-MeG). Hindered rotation was obsd. in the case of the ternary complexes with 1-MeC, in D2O solns. persisting up to 90.degree.. A cis-trans isomerization takes place in soln., increasing with temp. The crystal structure of cis-[(NH3)2Pt(1-MeC)(Gly)](NO3) was detd.

ACCESSION NUMBER: 1991:669127 CAPLUS
DOCUMENT NUMBER: 115:269127
TITLE: Ternary complexes of cisplatin with amino acids and nucleobases. The crystal structure of cis-[(NH3)2Pt(1-MeC-N3)(Gly-N)](NO3).cntdot.2H2O
AUTHOR(S): Iakovidis, Akis; Hadjiliadis, Nick; Britten, James F.; Butler, Ian S.; Schwarz, Frank; Lippert, Bernhard
CORPORATE SOURCE: Dep. Chem., Univ. Ioannina, Ioannina, 45-110, Greece
SOURCE: Inorganica Chimica Acta (1991), 184(2), 209-20
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **75659-46-0**
RL: PRP (Properties)
(IR and Raman spectra of)

RN 75659-46-0 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



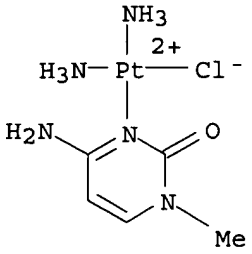
IT **75659-39-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amino acids)

RN 75659-39-1 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

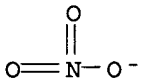
CM 1

CRN 75659-38-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



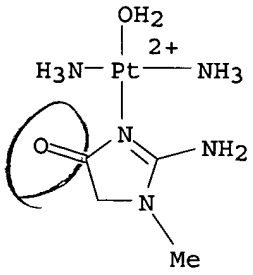
L7 ANSWER 44 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB With 195Pt NMR spectroscopy, several products formed in the 1:1 reaction at pH = 6-7 of cis-[Pt(NH3)2(H2O)2]2+ with creatinine (L) have been identified at pH 4 in aq. soln. The following products have been found: the heat-to-head and head-to-tail creatinine-bridged dimers [Pt2(NH3)4L2], [(NH3)2Pt(OH)2Pt(NH3)2]2+, cis-[Pt(NH3)2L]. They are closely related to the products that are obtained in analogous reactions of free and substituted pyrimidines. 13C NMR spectra of the complexes indicate large shifts for the C(3) and C(4) nuclei relative to the free ligand, indicating that the NH moiety within the creatinine ring, rather than the exocyclic one, is directly coordinated to the metal ion.

ACCESSION NUMBER: 1991:525570 CAPLUS
DOCUMENT NUMBER: 115:125570
TITLE: Platinum creatinine blues: reaction of cis-diamminediaquaplatinum(II) with creatinine studied by platinum-195 and carbon-13 NMR
AUTHOR(S): Geraldes, C. F. G. C.; Aragon-Salgado, M.; Martin-Gil, J.
CORPORATE SOURCE: Dep. Quim., Univ. Coimbra, Coimbra, 3000, Port.
SOURCE: Polyhedron (1991), 10(8), 799-803
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **135390-29-3P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by reaction of platinum ammine aqua complex with creatinine, NMR study of)

RN 135390-29-3 CAPLUS
CN Platinum(2+), (2-amino-1,5-dihydro-1-methyl-4H-imidazol-4-one-N3)diammineaqua-, (SP-4-3)- (9CI) (CA INDEX NAME)



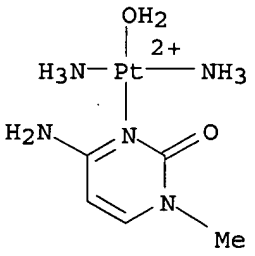
~~87~~ ANSWER 45 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB MO calcns. using the SC-MEH method have been carried out for the interaction of adenine, guanine, and cytosine and diamminecytosineplatinum (DCP) in various conformations. The results showed that the order of DCP binding to the DNA bases was guanine > adenine > cytosine and the stabilization energy of the cis-isomer was larger than that of the trans-isomer in the adenine-DCP complex system. Furthermore, Pt(II) binding to DNA bases markedly gives rise to a change of at. charge in the DNA base rings, which can explain anti-tumor activity of Pt complex.

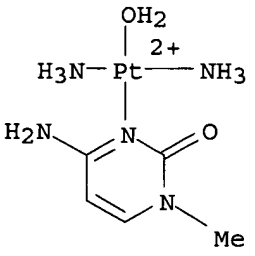
ACCESSION NUMBER: 1991:96943 CAPLUS
DOCUMENT NUMBER: 114:96943
TITLE: The electronic structure of platinum(II) interaction with DNA bases, adenine, guanine, and cytosine
AUTHOR(S): Kim, Ui Rak; Kim, Sang Hae; Boudreaux, Edward A.
CORPORATE SOURCE: Dep. Chem., Keimyung Univ., Taegu, 704-701, S. Korea
SOURCE: Taehan Hwahakhoe Chi (1990), 34(6), 539-47
CODEN: DHWHAB; ISSN: 0418-2472
DOCUMENT TYPE: Journal
LANGUAGE: Korean

IT **80662-70-0D**, nucleic acid base complexes **132201-90-2D**, nucleic acid base complexes
RL: PRP (Properties)
(electronic structure of, antitumor activity in relation to)

RN 80662-70-0 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 132201-90-2 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-2)- (9CI) (CA INDEX NAME)



L7 ANSWER 46 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Protonated and heteronuclear adducts and trans-L2PtX2 (L = NH3, NH2Me, HX = 1-methyluracil (HQ), or uridine) were prepd. and studied by spectroscopic methods and in 2 cases by x-ray crystallog. trans-(NH3)2PtQ2Ag2(NO3)2H2O.H2O (I) crystd. orthorhombic, space group Pna21, a 13.206(6), b 7.238(9), c 22.051(10) .ANG., Z = 4, R = 0.058, Rw = 0.063. I forms a polymeric structure with PtAg2 entities linked via O(4) sites of th 1-methyluracilato ligands. Pt is coordinated through N(3), the Ag centers have a mixed O(2), O(4) coordination. trans,trans,trans-[(NH3)2Pt(OH)2(HQ)2](NO3)2 (II) contains 2 N(3)-bound neutral 1-methyluracil ligands, hence rare tautomers of this model nucleobase. II crystallizes monoclinic, space group P21/n, a 7.098(1), b 10.395(1), c 13.295(2) .ANG., .beta. 91.88(2).degree., Z = 2, R = 0.059, Rw = 0.053. While the chem. leading to Pt(IV) oxidn. products from trans-L2PtX2 is similar to that of the cis-isomer, protonation as well as heteronuclear complex formation of trans-L2PtX2 is more difficult to accomplish than with the cis-isomer. This difference appears to be primarily of steric origin.

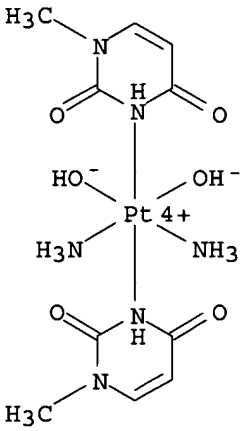
ACCESSION NUMBER: 1990:603810 CAPLUS
DOCUMENT NUMBER: 113:203810
TITLE: Coordination chemistry of trans-(H3N)2Pt(II) with uracil nucleobases. A comparison with cis-(H3N)2Pt(II)
AUTHOR(S): Dieter, Iris; Lippert, Bernhard; Schoellhorn, Helmut; Thewalt, Ulf
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-4600, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1990), 45(6), 731-40
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **129700-79-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure and deprotonation and reaction of, with chloride)

RN 129700-79-4 CAPLUS
CN Platinum(2+), diamminedihydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedione-.kappa.N3)-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

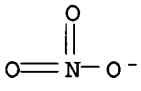
CM 1

CRN 129700-78-3
CMF C10 H20 N6 O6 Pt
CCI CCS



CM 2

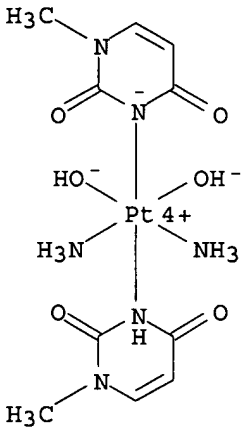
CRN 14797-55-8
CMF N O3



IT **129700-81-8P 129700-83-0P 129700-84-1P**
130039-07-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 129700-81-8 CAPLUS
CN Platinum(1+), diamminedihydroxy(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)(1-methyl-2,4(1H,3H)-pyrimidinedione-N3)-, (OC-6-13)-, nitrate (9CI) (CA INDEX NAME)

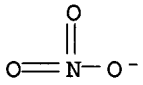
CM 1

CRN 129700-80-7
CMF C10 H19 N6 O6 Pt
CCI CCS

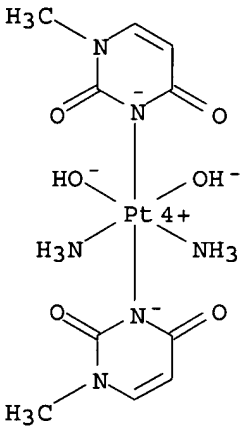


CM 2

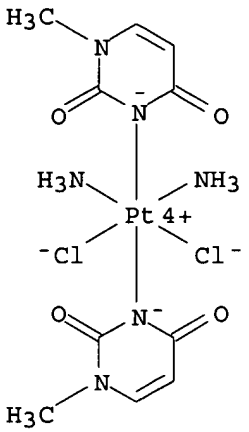
CRN 14797-55-8
CMF N O3



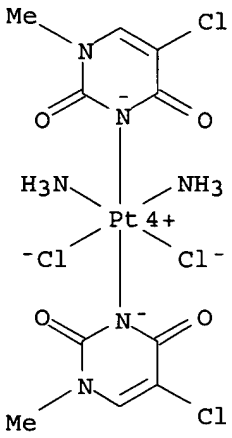
RN 129700-83-0 CAPLUS
CN Platinum, diamminedihydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-12)- (9CI) (CA INDEX NAME)



RN 129700-84-1 CAPLUS
CN Platinum, diamminedichlorobis(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-12)- (9CI) (CA INDEX NAME)



RN 130039-07-5 CAPLUS
CN Platinum, diamminedichlorobis(5-chloro-1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-12)- (9CI) (CA INDEX NAME)



L7 ANSWER 47 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The formation and properties of isomeric complexes of cis-(NH3)2Pt(II) contg. the model nucleobase 1-methylcytosine (1-MeCH), and glycine (glyH) are reported. Depending on the pH, different protonation states of the amino acid and nucleobase are present. In acidic medium, cis-[(NH3)2Pt(1-MeCH)(H2O)]2+ initially forms with glyH cis-[(NH3)2Pt(1-MeCH)(glyH-O)]2+ (I) which slowly at pH 2-3 and faster at pH 4-5 converts into cis-[(NH3)2Pt(1-MeCH)(gly-N)]+ (II). II is protonated to give the glyH-N species with a pKa .simeq. 2.8 and deprotonated at the NH2 group of 1-MeCH with a Ka .simeq. 12.5-13. Deprotonation of I was not detected at pH .ltoreq.6, at which point conversion I .fwdarw. II was complete. II was prepd. and isolated as the nitrate salt via 2 different routes, starting either from cis-[(NH3)2Pt(gly-N,O)]+ or from cis-[(NH3)2Pt(1-MeCH)(H2O)]2+. Only the second way led to both O- and N-bound glycine complexes. In the absence of glyH, cis-[(NH3)2Pt(1-MeCH)(H2O)]2+ undergoes a condensation reaction initially to cis-[(NH3)2Pt(1-MeCH)(OH)Pt(1-MeCH)(NH3)2]3+ and slowly to cis-[(NH3)2Pt(1-MeCH)2Pt(NH3)2]2+. Analogs of II with 9-methylguanine (9-MeGH) instead of 1-MeCH as well as mixed 1-MeCH, alanine and mixed 9-MeGH, alanine complexes have also been prepd. and isolated.

ACCESSION NUMBER: 1990:583568 CAPLUS
DOCUMENT NUMBER: 113:183568
TITLE: Ternary complexes of cis-(NH3)2Pt(II) with model nucleobases (1-methylcytosine, 9-methylguanine) and N- and O-bound amino acids (gly, ala)
AUTHOR(S): Schwarz, Frank; Lippert, Bernhard; Iakovidis, Akis; Hadjiliadis, Nick
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-4600, Germany
SOURCE: Inorganica Chimica Acta (1990), 168(2), 275-81
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

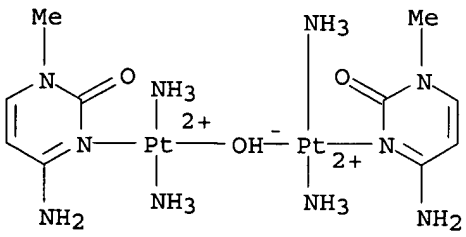
IT **129905-73-3P 129941-54-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 129905-73-3 CAPLUS

CN Platinum(3+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-N3)tetraammine-.mu.-hydroxydi-, stereoisomer, trinitrate (9CI) (CA INDEX NAME)

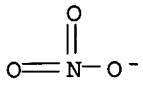
CM 1

CRN 129905-72-2
CMF C10 H27 N10 O3 Pt2
CCI CCS



CM 2

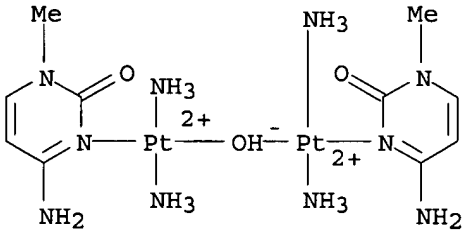
CRN 14797-55-8
CMF N O3



RN 129941-54-4 CAPLUS
CN Platinum(3+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-N3)tetraammine-.mu.-hydroxydi-, stereoisomer, triperchlorate (9CI) (CA INDEX NAME)

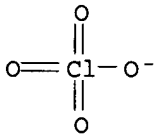
CM 1

CRN 129905-72-2
CMF C10 H27 N10 O3 Pt2
CCI CCS

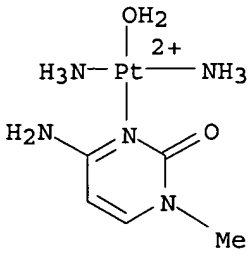


CM 2

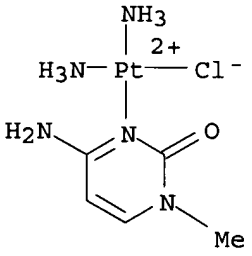
CRN 14797-73-0
CMF Cl O4



IT **80662-70-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glycine)
RN 80662-70-0 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)- (9CI) (CA INDEX NAME)



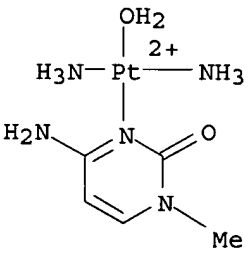
IT **75659-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silver nitrate followed by reaction with glycine)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **80662-71-1 98874-75-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(self reaction of, in alk. soln., binuclear complex by)
RN 80662-71-1 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)-, dinitrate (9CI) (CA INDEX NAME)

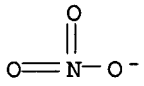
CM 1

CRN 80662-70-0
CMF C5 H15 N5 O2 Pt
CCI CCS



CM 2

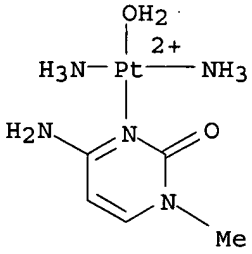
CRN 14797-55-8
CMF N O3



RN 98874-75-0 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)

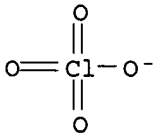
CM 1

CRN 80662-70-0
CMF C5 H15 N5 O2 Pt
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



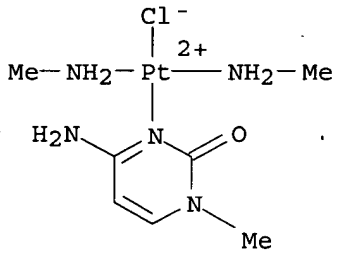
L7 ANSWER 48 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB trans-[(NH2Me)2Pt(1-MeCH)Cl]Cl.H2O (I) and trans-[(NH2Me)2Pt(1-MeCH)(gly)]NO3.2H2O (II; 1-MeCH = 1-methylcytosine, Hgly = glycine) were prepd. and are considered to be a precursor (I) and a product (II) of a hypothetical crosslinking reaction of a trans-diamineplatinum(II) moiety with a nucleic acid and the amino terminus of a protein, peptide, or amino acid. I crystd. in the space group P.hivin.1, Z = 2, R = 0.037, Rw = 0.042. II crystd. in the space group P.hivin.1, Z = 2, R = 0.025, Rw = 0.026. PH-dependent 1H NMR spectra of II in D2O have been recorded at 0.4 < pH < 13.5 and are indicative of two acid/base equil.with pKa .apprxeq.2.5 and 12.5.

ACCESSION NUMBER: 1990:544028 CAPLUS
DOCUMENT NUMBER: 113:144028
TITLE: Mixed nucleobase, amino acid complexes of platinum(II). Preparation and x-ray structure of trans-[(CH3NH2)2Pt(1-MeC-N3)(gly-N)]NO3.2H2O and its precursor trans-[(CH3NH2)2Pt(1-MeC-N3)Cl]Cl.H2O
AUTHOR(S): Pesch, Ferdinand J.; Preut, Hans; Lippert, Bernhard
CORPORATE SOURCE: Fachber. Chem., Univ. Dortmund, Dortmund, D-4600, Germany
SOURCE: Inorganica Chimica Acta (1990), 169(2), 195-200
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **129232-51-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and crystal structure and reaction of, with glycine and silver nitrate)

RN 129232-51-5 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)chlorobis(methanamine)-, chloride, monohydrate, (SP-4-2)- (9CI) (CA INDEX NAME)



Cl⁻

H2O

L7 ANSWER 49 OF 87 CAPLUS COPYRIGHT 2003 ACS

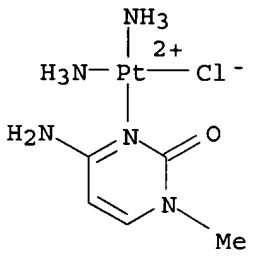
AB trans-[Pt(NH3)2(mec)Cl]Cl.1.5H2O (mec-1-methylcytosine), prepd. from trans-[Pt(NH3)2Cl2] and mec, is converted to trans-[Pt(NH3)2Cl2] and 2 rotamers of trans-[Pt(NH3)2(mec)2]Cl2 according to 1H NMR data. Similarly trans-[Pt(MeNH2)2(mec)Cl]Cl was converted to trans-[Pt(NH3)2Cl2] and trans-[Pt(MeNH2)2(mec)2]Cl2. Initially mec is displaced from trans-[PtL2(mec)Cl]+ (L = NH3, MeNH2) and subsequently coordinates to trans-[PtL2(mec)Cl]+ to give inert trans-[PtL2(mec)2]Cl2. The coordination behavior of trans-[Pt(NH3)2Cl2] toward DNA is discussed in terms of these results.

ACCESSION NUMBER: 1990:490210 CAPLUS
DOCUMENT NUMBER: 113:90210
TITLE: Nucleobase displacement from trans-diamineplatinum(II) complexes. A rationale for the inactivity of trans-DDP as an antitumor agent?
AUTHOR(S): Krizanovic, Olga; Pesch, Ferdinand J.; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-4600, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1989), 165(2), 145-6
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **98920-59-3P**, trans-Diaminechloro(1-methylcytosine)platinum(1+) monochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redistribution reaction of)

RN 98920-59-3 CAPLUS

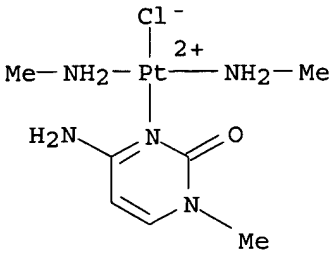
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **128636-28-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(redistribution reaction of)

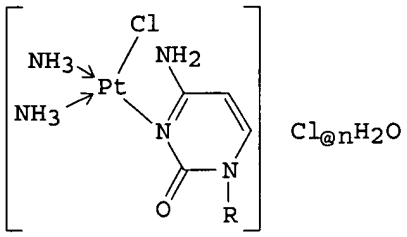
RN 128636-28-2 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)chlorobis(methanamine)-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



● Cl⁻

ANSWER 50 OF 87 CAPLUS COPYRIGHT 2003 ACS



I

AB Compds. of the formula I, where R = H and n = 1 or R = D-ribose and n = 2, exhibit antitumor activity.

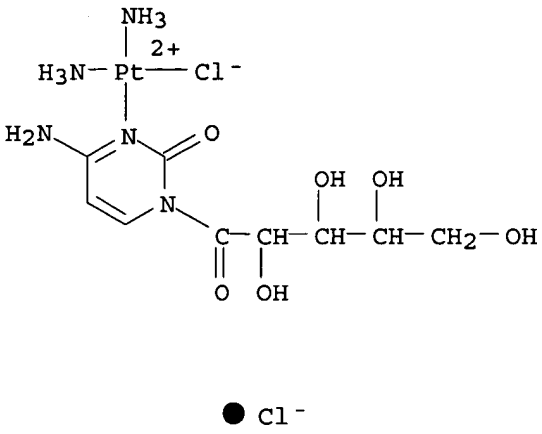
ACCESSION NUMBER: 1990:228669 CAPLUS
DOCUMENT NUMBER: 112:228669
TITLE: Chloro-cis-diamnine(aminooxypyrimidine)platinum(II) chlorides displaying antitumor activity
INVENTOR(S): Stetsenko, A. N.; Yakovlev, K. I.; Alekseeva, G. M.; Konovalova, A. L.; Presnov, M. A.
PATENT ASSIGNEE(S): Leningrad Chemical-Pharmaceutical Institute, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1989, (29), 285. CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1085209	A1	19890807	SU 1982-3472411	19820715

PRIORITY APPLN. INFO.: SU 1982-3472411 19820715

IT **127161-91-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(antitumor agent)

RN 127161-91-5 CAPLUS
CN Platinum(1+), (4-amino-1-D-ribonoyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



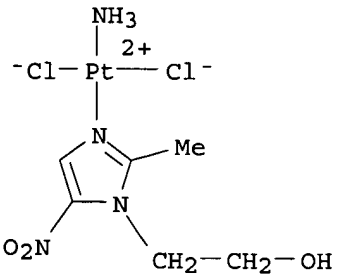
L7 ANSWER 51 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB There is increasing interest in compds. which show selective toxicity to the resistant hypoxic portions of tumors. Cisplatin does not generally show preferential toxicity in hypoxic cells, whereas nitroimidazoles do. It is proposed that attachment of a nitroimidazole could add a degree of hypoxic selectivity to Pt agents. Pt complexes contg. one nitroimidazole ligand bind to DNA and show higher toxicity in hypoxic than aerobic CHO cells. cis And trans isomers of complexes with misonidazole (a 2-nitroimidazole) and metronidazole (a 5-nitroimidazole) are compared with respect to binding to DNA (approx. the same), redn. potential (trans miso > cis miso > cis metro > trans metro), and toxicity (trans > cis meso, cis > trans metro, with trans miso .apprx. cis metro in hypoxia, despite significantly different redn. potentials). The effect of platination on nitroimidazole toxicity is not entirely explained by DNA binding and increased redn. potential. These compds. do not exhibit cross resistance with cisplatin in L1210 resistant cells. This factor, their selectivity for hypoxia, and preliminary results in vivo indicating potentiation of antitumor activity by the vasoactive compd., hydralazine, which increases tumor hypoxia, suggest further development of these compds. for use in tumors with resistant hypoxic portions.

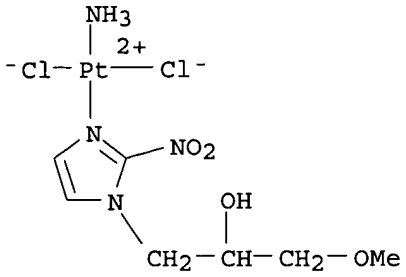
ACCESSION NUMBER: 1990:210664 CAPLUS
DOCUMENT NUMBER: 112:210664
TITLE: Toxicity of [PtCl2(NH3)L] in hypoxia; L = misonidazole or metronidazole
AUTHOR(S): Skov, K. A.; Adomat, H.; Chaplin, D. J.; Farrell, N. P.
CORPORATE SOURCE: Med. Biophys. Unit, BC Cancer Res. Cent., Vancouver, BC, V5Z 1L3, Can.
SOURCE: Anti-Cancer Drug Design (1990), 5(1), 121-8
CODEN: ACDDEA; ISSN: 0266-9536
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **110321-22-7 112198-62-6 114532-23-9 121350-06-9**
RL: PRP (Properties)
(cytotoxicity of, in hypoxia, structure in relation to)

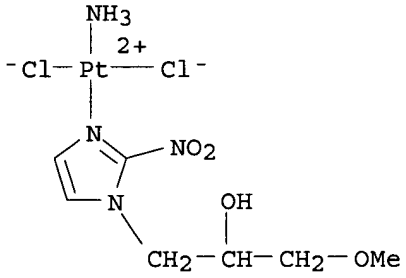
RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



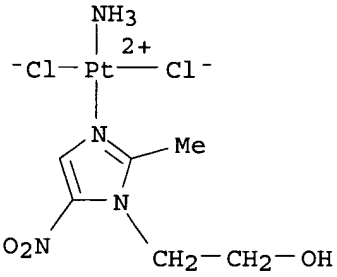
RN 112198-62-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 114532-23-9 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 121350-06-9 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-1)- (9CI) (CA INDEX NAME)



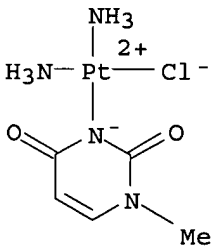
ANSWER 52 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB {[(Dien)Pt]2(L-N7,N1)}(ClO4)3.2H2O (I; dien = diethylenetriamine; HL = 9-methylguanine) and cis-[(NH3)2Pt(L-N1,N7)(L1-N3)Pt(dien)](ClO4)2.2.5H2O (II; HL1 = 1-methyluracil) were prepd. from [(dien)Pt(HL-N7)]2+ (III) and characterized by x-ray structural anal. I is monoclinic, space group C2/c, Z = 8. II is triclinic, space group P.hivin.1, Z = 2. In both cations, a (dien)PtII entity is coordinated to the guanine via N7, whereas the N1 position is either occupied by a (dien)PtII for I or a cis-(NH3)2PtL1 for the II residue. Coordination of the Pt at N1 takes place from III under virtually physiol. pH conditions. II represents an example of a hypothetical DNA cross-link of cisplatin with N1 of a purine and N3 of a pyrimidine, 2 sites normally in the interior of a DNA double helix. Both nucleobases adopt a head-head orientation, thus making II a realistic model of a guanine, thymine cross-link. The large dihedral angle of 102.degree. between the 2 bases and the long sepn. of 9.5 .ANG. between the alkyl groups of both bases point toward a DNA distortion, which, if realized, should exceed that of the L,L adduct at the DNA periphery. In slightly acidic medium, III interacts with Ag+ without deprotonation at N1 but rather Ag+ binding to N3.

ACCESSION NUMBER: 1990:171037 CAPLUS
DOCUMENT NUMBER: 112:171037
TITLE: Platinum(II) binding to N7 and N1 of guanine and a model for a purine-N1,pyrimidine-N3 cross-link of cisplatin in the interior of a DNA duplex
AUTHOR(S): Frommer, Gudrun; Schoellhorn, Helmut; Thewalt, Ulf; Lippert, Bernhard
CORPORATE SOURCE: Fachbereich Chem., Univ. Dortmund, Dortmund, D-4600, Germany
SOURCE: Inorganic Chemistry (1990), 29(7), 1417-22
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with platinum guanine diethylenetriamine complex)

RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



L7 ANSWER 53 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Square planar Pt(II) complexes are described of the formula [PtX2(NR2H)L] (I) or [PtX(NR2H)2L]+Y- (II) [X, Y- = a monovalent biol. acceptable anion (X2 in I may also be a divalent biol. acceptable anion); R = H or C1-8 alkyl; R2 = a morpholino or piperidino residue; L = a radiosensitizing mononitro-substituted arom. ligand with .gtoreq.1 heterocyclic N and/or substituent amine]. These complexes bind to DNA and sensitize hypoxic tumors to radiation; they are useful chemotherapeutic agents. cis-I (R = H; X = Cl; L = misonidazole) (cis-III) was prepd. by reaction of 1 equiv of misonidazole with K[PtCl3(NH3)] and treatment of the residue with Et2O. Treatment of cis-III with EtOH yielded trans-III. Chinese hamster ovary cells were incubated with III (100 .mu.mol/dm3) for 1 h at 37.degree. to allow binding to DNA prior to radiation. By use of a known method, radiosensitization of the cells was obsd.

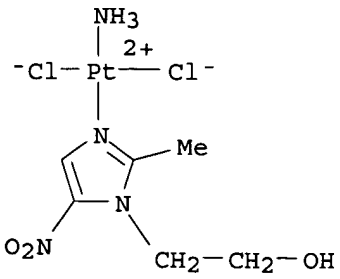
ACCESSION NUMBER: 1989:453447 CAPLUS
DOCUMENT NUMBER: 111:53447
TITLE: Platinum(II) complexes with one radiosensitizing ligand useful in tumor therapy
INVENTOR(S): Skov, Kirsten A.; Farrell, Nicholas P.; Chaplin, David J.
PATENT ASSIGNEE(S): British Columbia Cancer Foundation, Can.
SOURCE: Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 287317	A2	19881019	EP 1988-303258	19880412
EP 287317	A3	19890208		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4921963	A	19900501	US 1987-37498	19870413
JP 01052788	A2	19890228	JP 1988-92608	19880413
CA 1299179	A1	19920421	CA 1988-564082	19880413
US 5026694	A	19910625	US 1989-374356	19890630

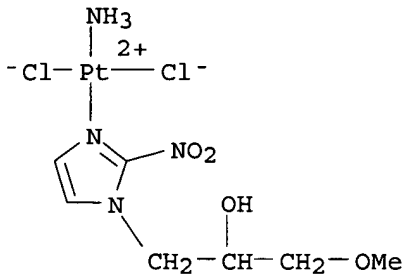
PRIORITY APPLN. INFO.: US 1987-37498 19870413
OTHER SOURCE(S): MARPAT 111:53447

IT **110321-22-7 112198-62-6 114532-23-9**
121281-51-4 121350-02-5 121350-03-6
121350-04-7 121350-06-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(as radiosensitizer, for neoplasm treatment)

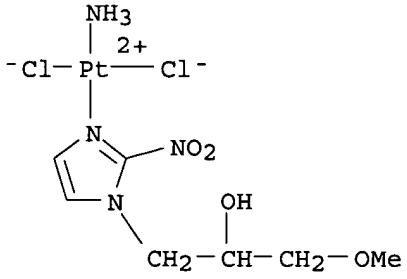
RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



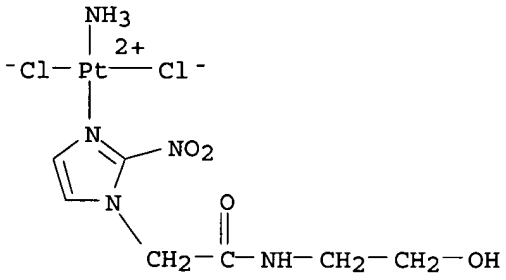
RN 112198-62-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



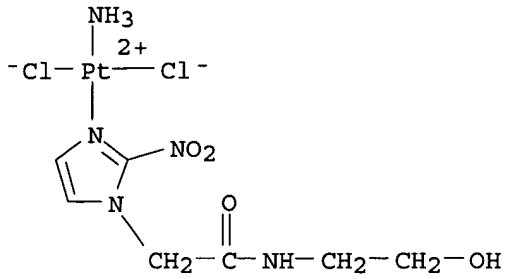
RN 114532-23-9 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-1)- (9CI) (CA INDEX NAME)



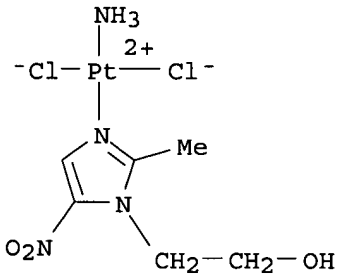
RN 121281-51-4 CAPLUS
CN Platinum, amminedichloro[N-(2-hydroxyethyl)-2-nitro-1H-imidazole-1-acetamide-N3]-, (SP-4-1)- (9CI) (CA INDEX NAME)



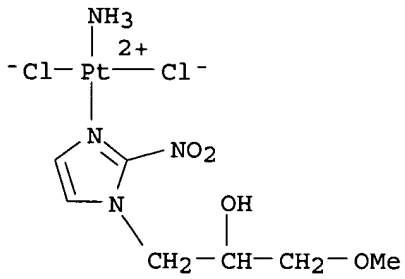
RN 121350-02-5 CAPLUS
CN Platinum, amminedichloro[N-(2-hydroxyethyl)-2-nitro-1H-imidazole-1-acetamide-N3]- (9CI) (CA INDEX NAME)



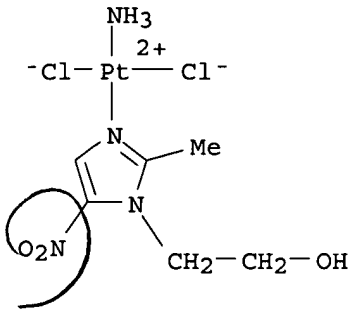
RN 121350-03-6 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-(9CI) (CA INDEX NAME)



RN 121350-04-7 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]- (9CI) (CA INDEX NAME)



RN 121350-06-9 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-1)- (9CI) (CA INDEX NAME)



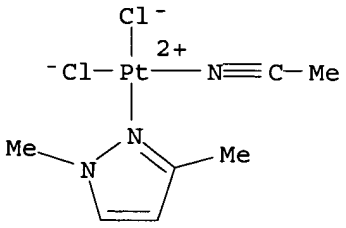
ANSWER 54 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Et4N[Pt(MeCN)Cl3] (I) reacted with pyridine in aq. soln. to give trans-Pt(MeCN)pyCl2 (II) whereas I reacted with other amines to give cis- and trans-Pt(MeCN)LCl2 (III; L = benzimidazole, 2,5-dimethylpyrazole, PhNH2, p-anisidine). In Me2CO or MeCN trans-II is in equil. with cis-II. The formation of trans-III and the isomerization of trans-II confirm the high dynamic trans effect of MeCN in Pt(II) complexes. I is monoclinic, space group P21/c, with a 7.335(3) b 17.352(3), c 12.942(3) .ANG., .beta. 101.92(4).degree., dc = 1.984(3) g cm-3, Z = 4. The Pt-Cl bond for the Cl trans to MeCN is 2.262 .ANG. whereas the Pt-Cl bonds for cis Cl's are 2.293 and 2.301 .ANG., which indicate the high static trans effect of the Cl in comparison to MeCN. cis-Pt(MeCN)2Cl2 reacted with MCl to give M[Pt(MeCN)Cl3] (M = PPh4+, Ph3PCH2Ph+, AsPh4+, Et4N+, Bu4N+). Ph3PCH2Ph[Pt(MeCN)Cl3] was also obtained by dissoln. of (Ph3PCH2Ph)2[Pt2(.mu.-Cl)2Cl4] in MeCN or by the reaction of (Ph3PCH2Ph)2[Pt(NO2)Cl3] with Ti2(SO4)3 in MeCN-H2O.

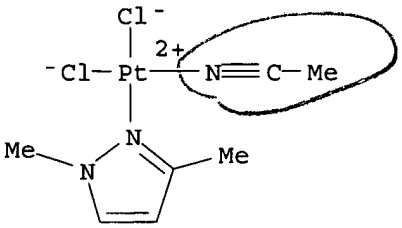
ACCESSION NUMBER: 1989:184755 CAPLUS
DOCUMENT NUMBER: 110:184755
TITLE: Dynamic and static trans effect of acetonitrile in platinum(II) complexes
AUTHOR(S): Krol, I. A.; Kukushkin, V. Yu.; Starikova, Z. A.; Tkachuk, V. M.; Zhadanov, B. V.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Obshchei Khimii (1988), 58(11), 2625-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **119341-13-8P**, cis-(Acetonitrile)dichloro(2,5-dimethylpyrazole)platinum **119433-34-0P**, trans-(Acetonitrile)dichloro(2,5-dimethylpyrazole)platinum
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 119341-13-8 CAPLUS
CN Platinum, (acetonitrile)dichloro(1,3-dimethyl-1H-pyrazole-N2)-, (SP-4-3)-(9CI) (CA INDEX NAME)



RN 119433-34-0 CAPLUS
CN Platinum, (acetonitrile)dichloro(1,3-dimethyl-1H-pyrazole-N2)-, (SP-4-1)-(9CI) (CA INDEX NAME)


Cl -
2+
- Cl— Pt— N≡C— Me
N
Me
N
Me

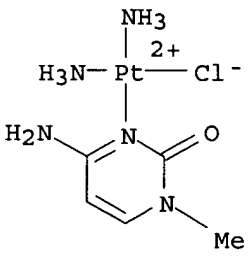
L7 ANSWER 55 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A series of 32 cis-[PtA2(Am)Cl]+ (A = NH3 or Me2CHNH2; A2 = en or 1,2-diaminocyclohexane) amine and Am = either a heterocyclic amine based on a pyridine, pyrimidine, purine, piperidine, or a satd. amine (RNH2) ligand) was prepd. and screened against in vivo murine tumor models. Each compd. was tested against Sarcoma 180 ascites (S180a) in mice, with 20 members of the series showing activity (ILS >50%). Antitumor activity also was demonstrated in 4 of 16 compds. tested in the L1210 murine leukemia model (ILS > 25%) and in 3 of 3 tested in the P388 murine leukemia model (ILS > 30%). The most active and potent analog of the series were obtained when A was NH3 and Am was pyridine, methylpyridine, bromopyridine, 4-chloropyridine, N3-cytosine, or N7-2'-deoxyguanosine. Complexes contg. chelating and satd. amine ligands (A), as well as 2 trans isomers of active cis analogs (trans-[Pt(NH3)2(Am)Cl]+ (Am = py or methylpyridine)), were inactive in the S180a screen. All complexes were characterized by elemental anal., HPLC, and 195Pt NMR spectroscopy, and the structure of cis-[Pt(NH3)2(Am)Cl]Cl (Am = N3-cytosine) was detd. by using single-crystal x-ray diffraction methods (monoclinic, P21/c, a 6.6708(4), b 7.6446(5), c 20.340(2) .ANG., .beta. 98.470(5).degree., Z = 4, R1 = 0.038, and R2 = 0.045). While members of this series of compds. demonstrate antitumor activity in vivo, these new agents are not classical analogs of cisplatin (i.e. cis-[PtA2X2] complexes), as they contain 3 N donors and only 1 leaving group. The results of these studies suggest that further work should be conducted to better define the limits of the structure-activity relationships among Pt(II) complexes.

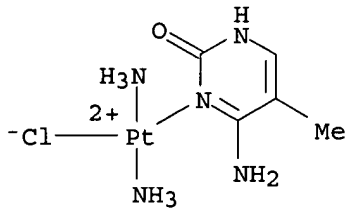
ACCESSION NUMBER: 1989:32871 CAPLUS
DOCUMENT NUMBER: 110:32871
TITLE: Chemical and biological properties of a new series of cis-diammineplatinum(II) antitumor agents containing three nitrogen donors: cis-[Pt(NH3)2(N-donor) Cl]+
AUTHOR(S): Hollis, L. Steven; Amundsen, Alan R.; Stern, Eric W.
CORPORATE SOURCE: Engelhard Corp., Edison, NJ, 08818, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(1), 128-36
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **75659-46-0P 117251-19-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and platinum-195 NMR and antitumor activity of)

RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 117251-19-1 CAPLUS
CN Platinum(1+), (4-amino-5-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



ANSWER 56 OF 87 CAPLUS COPYRIGHT 2003 ACS

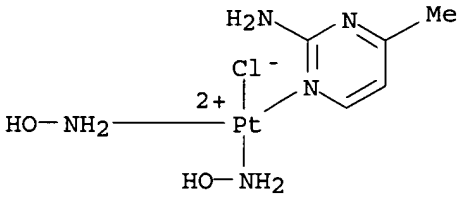
AB trans-[Pt(NH2OH)2LCl]Cl (L = py, 2-, 3-, 4-picoline, 2- and 4-aminopyridine, nicotinamide, isonicotinamide, 2-aminopyrimidine, 2-amino-4-methylpyrimidine, quinoline) were prepd. The effect of the nature of L was studied on the acidity of NH2OH in the complexes and on the reducibility of Pt in the complexes in the polarog. redn. process. The nature of L does not significantly affect acid dissocn. const. of coordinated NH2OH. The polarograms of these complexes are characterized by 2 waves, the 1st of which is assigned to redn. of the complex, occurring via a nonreversible 2-electron diffused-kinetic, complex adsorption process. The 2nd wave is due to the kinetic redn. of H+. The nicotinamide and isonicotinamide complexes are the easiest to reduce because of participation of the carbonyl group.

ACCESSION NUMBER: 1988:642998 CAPLUS
DOCUMENT NUMBER: 109:242998
TITLE: Physicochemical studies of platinum(II) hydroxylamine-containing complexes with nitrogen-containing heterocyclic ligands
AUTHOR(S): Tikhonova, L. S.; Stetsenko, A. I.
CORPORATE SOURCE: Leningr. Khim.-Farm. Inst., Leningrad, USSR
SOURCE: Zhurnal Neorganicheskoi Khimii (1988), 33(9), 2324-7
CODEN: ZNOKAQ; ISSN: 0044-457X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **117767-90-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acid dissocn. const. of)

RN 117767-90-5 CAPLUS

CN Platinum(1+), chlorobis(hydroxylamine-N)(4-methyl-2-pyrimidinamine-N1)-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



⊙ Cl -

L7 ANSWER 57 OF 87 CAPLUS COPYRIGHT 2003 ACS

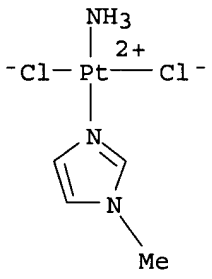
AB cis-Pt(NH3)LCl2 (L = thiazole, 2-bromothiazole, benzothiazole, 2,1,3-benzothiadiazole, 1,2,3-benzothiadiazole, imidazole, 1-methylimidazole) were prepd. The complexes were characterized by IR and UV-visible spectroscopy, 1H NMR and elemental analyses. The thiazoles and benzothiazoles were coordinated through the N heteroatom. Both the benzothiadiazoles were coordinated through S. Several of the complexes showed significant cytotoxic activity.

ACCESSION NUMBER: 1988:215259 CAPLUS
DOCUMENT NUMBER: 108:215259
TITLE: Synthesis and characterization of new platinum(II) complexes containing thiazole and imidazole donors
AUTHOR(S): Muir, Mariel M.; Cadiz, Mayra E.; Baez, Adriana
CORPORATE SOURCE: Dep. Chem., Univ. Puerto Rico, Rio Piedras, 00932, P. R.
SOURCE: Inorganica Chimica Acta (1988), 151(3), 209-13
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **114487-38-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

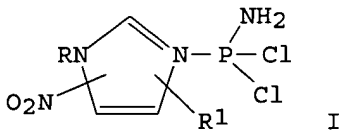
RN 114487-38-6 CAPLUS

CN Platinum, amminedichloro(1-methyl-1H-imidazole-.kappa.N3)-, (SP-4-3)-(9CI) (CA INDEX NAME)



L7 ANSWER 58 OF 87 CAPLUS COPYRIGHT 2003 ACS

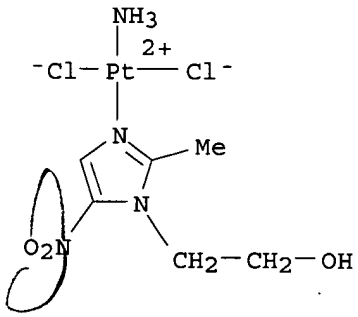
GI



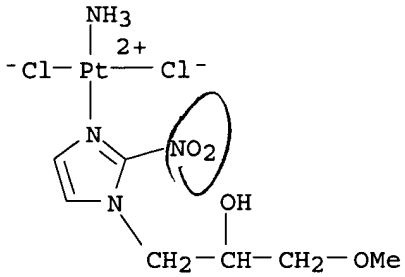
I

AB The prepn. and characterization of cis-[PtCl2(NH3)(misonidazole)] (I; R = CH2CH(OH)CH2OMe, R' = NO2) and cis-[PtCl2(NH3)(metronidazole)] (I; R = CH2CH2OH, R' = Me) are described and their binding to DNA and radiosensitizing activity were examd. Both complexes showed considerable DNA binding and had greater radiosensitizing activity then their bis analogs. The results indicate that radiosensitizing ligands can be targeted to DNA by complexation with Pt.

ACCESSION NUMBER: 1988:108927 CAPLUS
DOCUMENT NUMBER: 108:108927
TITLE: Radiosensitizers targeted to DNA using platinum. Synthesis, characterization, and DNA binding of cis-[PtCl2(NH3)(nitroimidazole)]
AUTHOR(S): Farrell, Nicholas; Skov, Kirsten A.
CORPORATE SOURCE: Dep. Chem., Univ. Vermont, Burlington, VT, 05405, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (13), 1043-4
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **110321-22-7P 112198-62-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and DNA binding and radiosensitizing efficacy of)
RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 112198-62-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



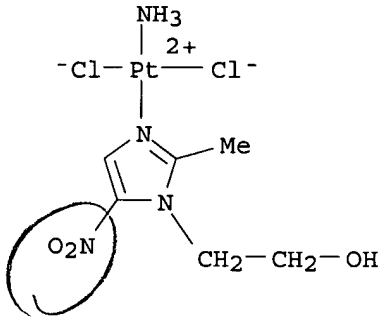
L7 ANSWER 59 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Complexes of general formula [PtCl2(NH3)L] with 1 radiosensitizing ligand per Pt are compared with ligand L alone, complexes with 2 radiosensitizers per Pt [PtCl2L2], and their analogs with NH3 ligands, with respect to radiosensitizing properties and toxicity in CHO cells. Radiosensitizing ligands, L, were misonidazole, metronidazole, 4(5)-nitroimidazole, and 2-amino-5-nitrothiazole, and the ammine analogs were cis- and trans-DDP [diamminedichloroplatinum(II)] and the monoammine, K[PtCl3(NH3)]. Results are related to a previous study on plasmid DNA binding by these series. The toxicity of the mono series [PtCl2(NH3)L], attributable to DNA binding, is much higher than the corresponding bis complexes, [PtCl2L2]. For L = misonidazole, toxicity is similar to the monoammine, but higher in hypoxic than in aerobic cells. trans-[PtCl2(NH3)-(misonidazole)] is more toxic than the cis isomer. Except for L = 4(5)-nitroimidazole, the complexes [PtCl2(NH3)L] are more toxic than L inm air and hypoxia. Hypoxic radiosensitization by the mono complexes is comparable to the monoammine and is not better than free sensitizers, again except for L = 4(5)-nitroimidazole. Significantly lower sensitization is obsd. in oxic cells. The bis complexes [PtCl2L2], which do not bind to DNA as well as the mono complexes, are less effective radiosensitizers and less toxic than the [PtCl2(NH3)L] series.

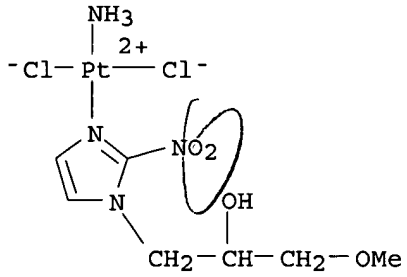
ACCESSION NUMBER: 1988:71355 CAPLUS
DOCUMENT NUMBER: 108:71355
TITLE: Platinum complexes with one radiosensitizing ligand [PtCl2(NH3) (sensitizer)]: radiosensitization and toxicity studies in vitro
AUTHOR(S): Skov, Kirsten A.; Farrell, Nicholas P.; Adomat, Hans
CORPORATE SOURCE: Med. Biophys. Unit, British Columbia Cancer Res. Cent., Vancouver, BC, V5Z 1L3, Can.
SOURCE: Radiation Research (1987), 112(2), 273-82
CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **110321-22-7 112198-62-6 114532-23-9**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (radiosensitizing activity and toxicity of, in CHO cells)

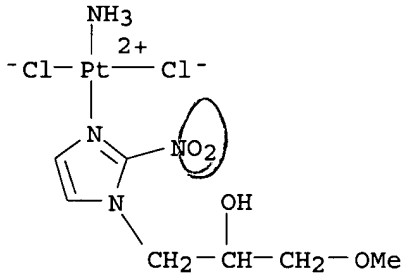
RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 112198-62-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 114532-23-9 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-2-nitro-1H-imidazole-1-ethanol-N3]-, (SP-4-1)- (9CI) (CA INDEX NAME)



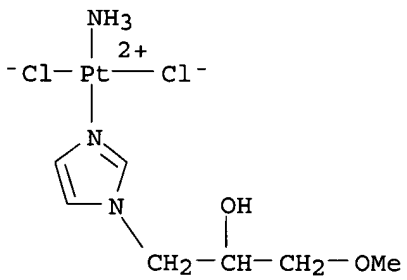
L7 ANSWER 60 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A simple and rapid method has been used to compare the binding of Pt complexes to DNA, in a relatively qual. manner. A compd. bound at or near the restriction site inhibits enzymic cleavage of DNA; inhibition of BamHI and EcoRI activities by complexes was assessed in this study using linearized pSV2-gpt plasmid. The particular interest was in DNA binding by complexes of Pt with known org. radiosensitizers (RS), to det. whether the Pt was able to target the RS to the DNA. Although the PT-RS complexes investigated themselves have moderate radiosensitizing ability (like the inorg. complexes, cis- or trans-DDP), none of the Pt-RS inhibit to the same extent as cis- or trans-DDP. However, there appears to be some correlation between enhanced radiosensitization by Pt-RS over Pt(RS)2, with the degree of Pt binding (as assessed by the assay). The results using isolated DNA suggest that not all complexes bind well (e.g., Pt with 2 RS ligands), but that in certain cases (e.g., Pt with only 1 RS), it is possible to target the drug to the DNA. An ammine or amine ligand may be required to target a radiosensitizer to DNA using Pt.

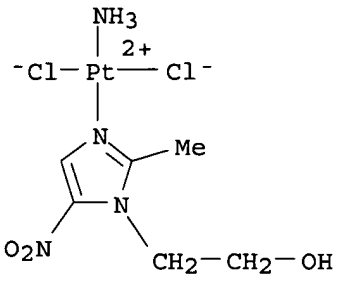
ACCESSION NUMBER: 1987:529989 CAPLUS
DOCUMENT NUMBER: 107:129989
TITLE: Assessment of DNA binding of platinum-radiosensitizer complexes by inhibition of restriction enzymes
AUTHOR(S): Skov, Kirsten A.; Adomat, Hans; Konway, Desmond C.; Farrell, Nicholas P.
CORPORATE SOURCE: Med. Biophys. Unit, British Columbia Cancer Res. Cent., Vancouver, BC, V5Z 1L3, Can.
SOURCE: Chemico-Biological Interactions (1987), 62(2), 117-29
CODEN: CBINA8; ISSN: 0009-2797
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **110321-21-6 110321-22-7**
RL: BIOL (Biological study)
(DNA binding of, restriction enzymes inhibition in assessment of, radiosensitization in relation to)

RN 110321-21-6 CAPLUS
CN Platinum, amminedichloro[.alpha.-(methoxymethyl)-1H-imidazole-1-ethanol-N3]-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 110321-22-7 CAPLUS
CN Platinum, amminedichloro(2-methyl-5-nitro-1H-imidazole-1-ethanol-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



L7 ANSWER 61 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The crystal structures are reported of 2 nucleobase complexes of cisplatin, cis-[(NH3)iPt(1-MeC)Cl]2[Pt(CN)4] (I) and cis-[(NH3)2Pt(1-MeC)2][Pt(CN)4].cntdot.2H2O (II), 1-MeC = 1-methylcytosine. I is monoclinic, space group P21/n, with a 17.576(7), b 10.916(5), c 6.846(3) .ANG., and .beta. 98.36(4).degree.; Z = 2. II is triclinic, space group P.hivin.1, with a 12.368(4), b 11.219(4), c 10.526(3) .ANG., .alpha. 109.12(4), .beta. 98.01(4), and .gamma. 113.65(4).degree.; Z = 1. The structures were refined to R = 0.051 (RW = 0.054) for I and R = 0.077 (RW = 0.077) for II. Pt coordination occurs in both complexes through the N(3) position of the cytosine ring. In II nucleobases are oriented head-to-tail. The structures are compared with related compds. contg. different counter anions. The at. coordinates are given.

ACCESSION NUMBER: 1986:600909 CAPLUS
DOCUMENT NUMBER: 105:200909
TITLE: Mono- and bis(1-methylcytosine) complexes of cisplatin: the crystal structures of cis-[(NH3)2Pt(1-MeC)Cl]2[Pt(CN)4] and cis-[(NH3)2Pt(1-MeC)2][Pt(CN)4].2H2O
AUTHOR(S): Schoellhorn, Helmut; Thewalt, Ulf; Raudaschl-Sieber, Gabriele; Lippert, Bernhard
CORPORATE SOURCE: Sekt. Roentgen- und Elektronenbeugung, Univ. Ulm, Ulm, D-79, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1986), 124(4), 207-11
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

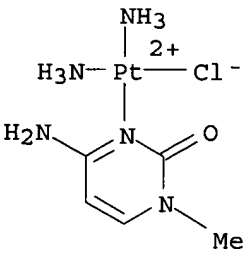
IT **96617-60-6**
RL: PRP (Properties)
(crystal structure of)

RN 96617-60-6 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, (SP-4-3)-, (SP-4-1)-tetrakis(cyano-C)platinate(2-) (2:1) (9CI) (CA INDEX NAME)

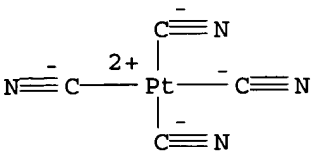
CM 1

CRN 75659-38-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 15004-88-3
CMF C4 N4 Pt
CCI CCS



L7 ANSWER 62 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A way is presented for estg. the geometry or rare nucleobase tautomers by (i) prepg. metal complexes of the rare tautomers, (ii) detg. the crystal structure of the metal complex as accurately as possible, and (iii) subtracting the effect of the metal on the ligand geometry. The prepn., crystal structures, and spectroscopic (1H NMR, Raman) properties are reported of 2 modifications of trans,trans,trans-[Pt(NH3)2(OH)2(1-MeC)2].2H2O (I; 1-MeC = 1-methylcytosine). Neutral 1-MeC ligands are coordinated to Pt through the deprotonated exocyclic N4' positions with N3 protonated. Thus the 1-MeC ligands are in the rare iminooxo tautomer form of cytosine. Modification A of I crystallizes in the triclinic space group P.hivin.1 with a 5.819(2), b 7.178(2), c 13.626(7) .ANG., .alpha. 90.72(4), .beta. 105.82(3), .gamma. 94.02(8).degree., Z = 1, R = 0.020, Rw(F) = 0.020 for 1911 independent reflections. Modification B of I crystallizes in the monoclinic space group P21/c with a 8.892(1), b 11.496(1), c 11.010(1) .ANG., .beta. 100.05(2).degree., Z = 2, R = 0.040, Rw(F) = 0.045 for 2525 independent reflections. The geometries of the 1-MeC ligands in A and B differ from that of the normal, uncomplexed 1-MeC tautomer with significant differences in C4-N4' and N1-C2 bond lengths (shorter in I), in N3-C4 and C2-N3 bond lengths (longer in I), as well as in ring angles at positions 2, 3, and 4. The effect of PtIV on the geometry of the cytosine ring is minimal and essentially restricted to the exocyclic imino group by slightly lengthening the C4-N4' bond. Formation of I occurs in 3 distinct steps, all of which were detected in soln., and the resp. species were isolated: (i) Pt coordination via N3, (ii) chelate formation through N3 and N4' with elimination of H2O from the complex, and (iii) addn. of H2O to the complex with reformation of Pt-OH and opening of the Pt-N3 bond. The acidity of the rare 1-MeC tautomer in its PtIV complexed form (deprotonation at N3) was detd. as .apprx.5.8 (pKa1) and .apprx.8.2 (pKa2).

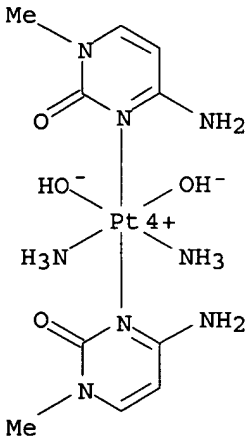
ACCESSION NUMBER: 1986:563817 CAPLUS
DOCUMENT NUMBER: 105:163817
TITLE: Metal-stabilized rare tautomers of nucleobases. 1. Iminooxo form of cytosine: formation through metal migration and estimation of the geometry of the free tautomer
AUTHOR(S): Lippert, Bernhard; Schoellhorn, Helmut; Thewalt, Ulf
CORPORATE SOURCE: Inst. Anorg. Anal. Chem., Univ. Freiburg, Freiburg, 7800, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1986), 108(21), 6616-21
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **101152-06-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(linkage isomerization, tautomerization via intermol. condensation and hydrolysis of)

RN 101152-06-1 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminedihydroxy-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

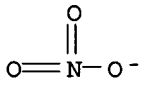
CM 1

CRN 101152-05-0
CMF C10 H22 N8 O4 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



L7 ANSWER 63 OF 87 CAPLUS COPYRIGHT 2003 ACS

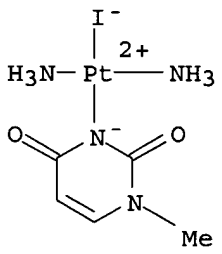
AB The prepn., compn., and the soln. behavior of [X(NH3)2PtL2Pt(NH3)2X1]Zn.mH2O (LH = 1-methyluracil (MuLH) or 5-chloro-1-methyluracil; X, X1 = NO2-, NO3-, Cl-, Br-, H2O or combinations thereof; Z = NO3-, Cl-, Br-; n = 2, 3) are reported. The compds. are obtained by chem. oxidn. (HNO3, HNO2, Cl2) of the head-tail Pt(II) dimer cis-[(NH3)2Pt(MuL)]2(NO3)2 or via ligand exchange reactions of the Pt(III) dimers, resp. The crystal structure of two modifications of [(ONO2)(NH3)2Pt(MuL)2Pt(NH3)2(OH2)] (NO3)3.mH2O (I; m = 3 and 2) were detd. The cations of both compds. are similar: Pt-Pt = 2.556(1), 2.560(1) .ANG.; Pt-OH2 = 2.18(1), 2.17(1) .ANG.; Pt-ONO2 = 2.14(1), 2.12(1) .ANG., resp. The structures are compared with the previously reported analog with X = NO2- and X1 = OH2. In aq. soln., axial X and X1 ligands such as Cl-, ONO2-, and NO2- readily undergo solvolysis with formation of [(OH2)(NH3)2PtL2Pt(NH3)2(OH2)]4+. PKa values of this complex were detd. as 3.5 and 6.7. At pH >2, diplatinum(III) complexes contg. nitro ligands are spontaneously reduced to the diplatinum(II) starting compd. In a secondary reaction, evolution of N is obsd., presumably formed between NH3 and NO2-. Diplatinum (III) complexes obtained through Cl2 oxidn. are special in that Cl2 also attacks the uracil ring with substitution of H5 by Cl. Iodine does not oxidize the diplatinum (II) precursor to the diplatinum (III) complex.

ACCESSION NUMBER: 1986:525953 CAPLUS
DOCUMENT NUMBER: 105:125953
TITLE: Diplatinum(III) complexes with bridging 1-methyluracil ligands in head-tail arrangement: synthesis, structures, and solution behavior
AUTHOR(S): Schoellhorn, Helmut; Eisenmann, Petra; Thewalt, Ulf; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganic Chemistry (1986), 25(19), 3384-91
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **103439-49-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 103439-49-2 CAPLUS

CN Platinum, diammineiodo(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



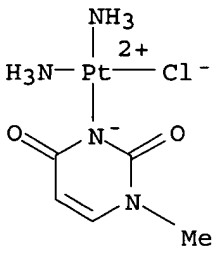
L7 ANSWER 64 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The PTL3 x-ray absorption spectra of a series of Pt compds. were recorded and their EXAFS analyzed to investigate the sensitivity of EXAFS to non-1st-shell Pt-Pt distances. The PtL3 EXAFS spectra of complexes formed between [(NH3)2Pt(OH)2Pt(NH3)2]2+ and calf thymus DNA were also recorded. Pt-Pt vectors were not detected in these spectra. When combined with the model compd. studies, this result rules out Pt dimer structures for the Pt-DNA complex which involve rigidly bridged, adjacent Pt atoms. Such structures based on dimeric bonding of a hydroxo dimer intermediate to DNA, were proposed as models for cisplatin antitumor activity. These types of models now seem unlikely.

ACCESSION NUMBER: 1986:523464 CAPLUS
DOCUMENT NUMBER: 105:123464
TITLE: PtL3 x-ray absorption studies of platinum model compounds and tetraammine-di-.mu.-hydroxodiplatinium(2+) bound to DNA
AUTHOR(S): Hitchcock, A. P.; Lock, C. J. L.; Lippert, B.
CORPORATE SOURCE: Dep. Chem., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Inorganica Chimica Acta (1986), 124(2), 101-14
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-78-2 85715-82-8**
RL: PRP (Properties)
(x-ray spectra of, DNA complex in relation to)

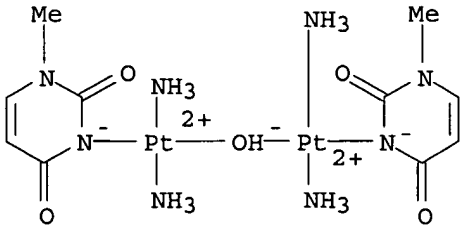
RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 85715-82-8 CAPLUS
CN Platinum(1+), tetraammine-.mu.-hydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)di-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

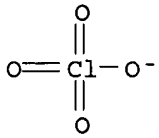
CM 1

CRN 85715-81-7
CMF C10 H23 N8 O5 Pt2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



L65 ANSWER 65 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Oxidn. of trans-[Pt(NH3)2(1-MeCH)2](NO3)2 (1-MeCH = 1-methylcytosine, bound to Pt through N3) with H2O2 gives trans,trans,trans-[Pt(NH3)2(1-MeCH)2(OH)2](NO3)2.2H2O (I). From strongly acidic HNO3 soln. I crystallizes in its monoprotonated form trans,trans-[Pt(NH3)2(1-MeCH)2(OH)(OH2)](NO3)3.3H2O (II). In weakly to moderately acidic medium (HNO3) or on warming, I is converted into trans-[Pt(NH3)2(1-MeCH)(1-MeC)(OH)](NO3)2.H2O (III) and trans,trans-[Pt(NH3)2(1-MeC)2](NO3)2.2H2O (IV), which contain 1 and 2 chelating, anionic 1-methylcytosinato ligands bound to the Pt through N3 and N4. The crystal structures of I, II, III, and IV were detd. The N3,N4 chelates in III and IV represent novel metal binding patterns with a cytosine nucleobase and at the same time the 1st examples of nucleobase chelates involving Pt. In these chelates, Pt-N3 and Pt-N4 distances are short and of comparable lengths, namely 1.969(13) and 2.032(16) .ANG. in II and 2.037(9) and 2.038(10) .ANG. in IV. The soln. behavior of I, II, III, and IV was studied by 1H NMR spectroscopy and potentiometric titrn. The pKa for the equil. II .dblharw. I + H+ is <1. Heating of I (II) in 3.5N HNO3 leads to displacement of 1-MeC. DCl (1N) causes substitution of OH ligands by Cl-, the substitution of the C5 proton of 1-MeC by Cl-, and eventually displacement of the modified nucleobase. Conversion of I into III and IV occurs in slight to moderate acidic soln. (pH 5.5-1.5). Isolated II (IV), when redissolved in H2O, equilibrates with I and IV (III). Two feasible ways of chelate formation are proposed, and the possible significance of 4-membered chelate rings in metal ions-nucleobase interactions is briefly discussed.

ACCESSION NUMBER: 1986:417097 CAPLUS
DOCUMENT NUMBER: 105:17097
TITLE: Unusual four-membered chelate rings of platinum(IV) with a cytosine nucleobase
AUTHOR(S): Schoellhorn, Helmut; Beyerle-Pfnuer, Rut; Thewalt, Ulf; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1986), 108(13), 3680-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

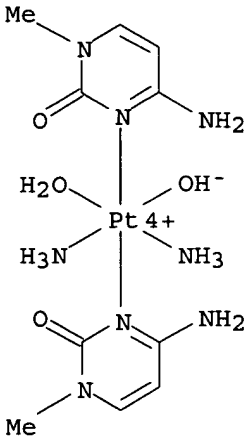
IT **102149-62-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)
RN 102149-62-2 CAPLUS
CN Platinum(3+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diammineaquahydroxy-, (OC-6-23)-, trinitrate, trihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 102149-61-1
CMF C10 H23 N8 O4 Pt . 2 N O3

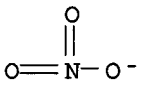
CM 2

CRN 102149-60-0
CMF C10 H23 N8 O4 Pt
CCI CCS

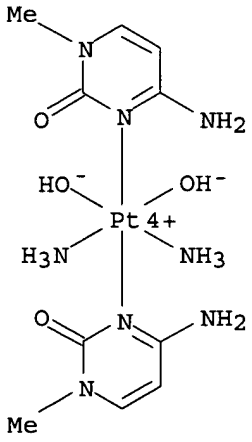


CM 3

CRN 14797-55-8
CMF N O3



IT **102210-45-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 102210-45-7 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminedihydroxy-, dichloride, (OC-6-12)- (9CI) (CA INDEX NAME)



2 Cl^-

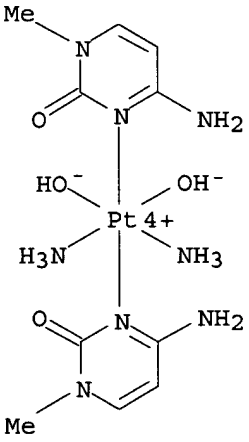
IT **102149-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., crystal structure and reaction with nitric acid)
RN 102149-59-7 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminedihydroxy-, (OC-6-12)-, dinitrate, dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 101152-06-1
CMF C10 H22 N8 O4 Pt . 2 N O3

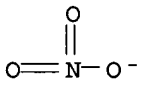
CM 2

CRN 101152-05-0
CMF C10 H22 N8 O4 Pt
CCI CCS



CM 3

CRN 14797-55-8
CMF N O3



L7 ANSWER 66 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The structure of [Pt(NH3)2L2](NO3)2.2H2O (I), prepd. from trans-[Pt(NH3)2(HL)2](NO3)2 (L = 1-methylcytosine) by oxidn. with H2O2 followed by warming in aq. HNO3, was detd. by x-ray crystallog. Crystals of I are monoclinic, space group P21/c, with a 7.230(3), b 10.576(4), c 13.186(2) .ANG., .beta. 100.92(3).degree., and d.(calcd.) = 2.138 g/cm3 for Z = 2. Results were refined to an R of 0.048 for 1419 reflections. I is the 1st example of anionic 1-methylcytosine acting as a chelating ligand through N-3 and N-4.

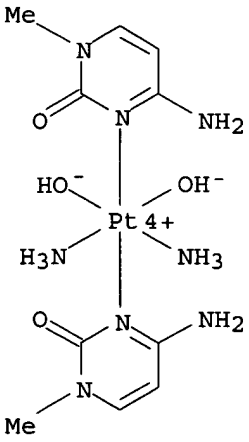
ACCESSION NUMBER: 1986:140933 CAPLUS
DOCUMENT NUMBER: 104:140933
TITLE: A novel metal binding mode of cytosine nucleobases: N(3),N(4) chelation
AUTHOR(S): Beyerle-Pfnuer, Rut; Schoellhorn, Helmut; Thewalt, Ulf; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
SOURCE: Journal of the Chemical Society, Chemical Communications (1985), (21), 1510-11
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **101152-06-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and dehydroxylation of)

RN 101152-06-1 CAPLUS
CN Platinum(2+), bis(4-amino-1-methyl-2(1H)-pyrimidinone-.kappa.N3)diamminedihydroxy-, (OC-6-12)-, dinitrate (9CI) (CA INDEX NAME)

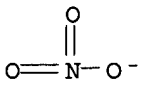
CM 1

CRN 101152-05-0
CMF C10 H22 N8 O4 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



L7 ANSWER 67 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB A series of mixed 9-methyladenine (9-MeA) and 1-methylcytosine (1-MeC) complexes of cis- and trans-(NH3)2Pt2+ were studied: cis-[(NH3)2Pt(9-MeA-N7)(1-MeC-N3)](ClO4)2.H2O (I), cis-[(NH3)2Pt(9-MeA-N1)(1-MeC-N3)]2+, cis-[(NH3)2(1-MeC-N3)Pt(9-MeA-N1,N7)Pt(1-MeC-N3)(NH3)2]4+, cis-[(NH3)2Pt(1-MeC-N3)(9-MeAH-N7)](ClO4)3.2H2O, trans-[(NH3)2Pt(1-MeC-N3)(9-MeA-N7)](ClO4)2 (II), trans-[(NH3)2Pt(1-MeC-N3)(9-MeA-N1)]2+, and trans-[(NH3)2(1-MeC-N3)Pt(9-MeA-N1,N7)Pt(1-MeC-N3)(NH3)2]4+ were isolated in cryst. form, and the crystal structures of I and II were detd. I is monoclinic space group C2/c, with a 30.526(5), b 8.380(2), c 20.925(4) .ANG., .beta. 121.92(1).degree., and Z = 8. II is monoclinic, space group P21/n, with a 13.234(2), b 11.406(2), c 14.620(4) .ANG., .beta. 93.78(2).degree., and Z = 4. On the basis of 4512 and 4784 reflections, resp., the structures were refined to R1 = 0.059, 0.068 for I and II, resp., and R2 = 0.074, 0.064 for I and II, resp. The cation of I has the 2 nucleobase planes approx. at right angles relative to the Pt coordination plane, with a moderately strong H bond between the exocyclic keto group of 1-MeC and the exocyclic amino group of 9-MeA, leading to a 91.6.degree. angle between the 2 base planes. In the trans isomer II, the 2 nucleobases are almost coplanar (dihedral angle 4.0.degree.) but again are perpendicular to the Pt coordination plane. While the cis-(NH3)2Pt(1-MeC) moiety reacts preferentially with the N7 position of 9-MeA, the trans-(NH3)2Pt(1-MeC) moiety prefers N1 over N7. Possible reasons for these differences in selectivity are discussed. 1H NMR spectra of the various complexes are compared and interpreted in terms of differences of diamagnetic anisotropies caused by ring-current effects. Relevant acid-base equil. for N7- and N1-platinated 9-MeA are reported and discussed briefly with regard to alterations in the base-pairing properties toward thymine.

ACCESSION NUMBER: 1985:604785 CAPLUS
DOCUMENT NUMBER: 103:204785
TITLE: Mixed-ligand cis and trans complexes of platinum(II) with cytosine and adenine nucleobases: crystal structures and solution studies of cis and trans isomers of (9-methyladenine-N7)(1-methylcytosine-N3)diammineplatinum(II) perchlorate. Different selectivities of aquadiammine(1-methylcytosine)platinum(II) isomers for N1 and N7 donor atoms of adenine
AUTHOR(S): Beyerle-Pfnur, Rut; Brown, Brenda; Faggiani, Romolo; Lippert, Bernhard; Lock, Colin J. L.
CORPORATE SOURCE: Inst. Inorg. Chem., Tech. Univ. Munich, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganic Chemistry (1985), 24(24), 4001-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

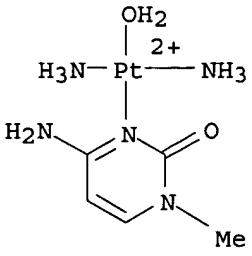
IT **98874-75-0 98920-59-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyladenine)

RN 98874-75-0 CAPLUS

CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)

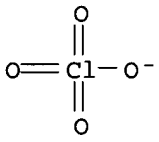
CM 1

CRN 80662-70-0
CMF C5 H15 N5 O2 Pt
CCI CCS

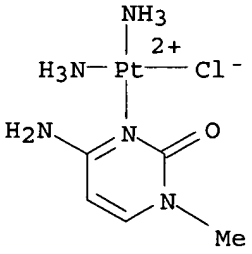


CM 2

CRN 14797-73-0
CMF Cl O4



RN 98920-59-3 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-
.kappa.N3)diamminechloro-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)



● Cl -

L7 ANSWER 68 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The behavior of a series of model nucleobase complexes of compn. cis-(NH3)2PtLX, trans-(NH3)2PtLX, (NH3)3PtL, trans-L2Pt(NH3)X, cis-[(NH3)2PtL]22+ (L = 1-methylcytosine (C), 9-ethylguanine (G), 9-methyladenine (A), deprotonated 1-methyluracil (U), deprotonated 1-methylthymine (T), or deprotonated 1-methylcytosine (C-H) and X = Cl-, OH-, H2O, or another nucleobase) toward CN- was studied in aq. soln. by spectroscopic (1H NMR, IR), preparative, and x-ray crystallog. methods. Monodentate bound G(N7), A(N7), and C(N3) bases were substituted rather quickly by CN- (half-life between minutes and 25 h), except from mixed-nucleobase complexes contg. one U or T bound through N3. In these complexes, the replacement of the bases was very slow (G,U) or no reaction occurred at all (C,U). Netierh cis-(NH3)2PtU2 [74539-69-8] nor cis-(NH3)2PtT2 [83350-97-4] showed reaction with CN-. Rather slow reaction was also obsd. with the dinuclear complex cis-[(NH3)2PtL]22+ with L = deprotonated 1-methylcytosine in head-tail orientation. These results are interpreted in terms of the kinetic stability of U-, T-, and (C-H)-contg. complexes as a consequence of steric shielding of Pt by the exocyclic oxygens ortho to the Pt coordination site. Reactions of selected nucleobase complexes with CN-, performed on a preparative scale, indicated that the first substitution of a ligand in the nucleobase complexes by CN- leads to a strong labilization of both cis and trans ligands and subsequently to formation of [Pt(CN)4]2- [15004-88-3]. If a large excess of CN- is avoided, and in certain cases of low soly., it is possible to isolate complexes of compn. cis-[(NH3)2PtLX]n[Pt(CN)4] (n = 1 or 2, depending on charge of X) and cis-(NH3)2LPt(NC)Pt(CN)3 with ionic and bridging [Pt(CN)4]2-, resp. The behavior of Pt-nucleobase complexes toward CN- is compared with that of simple Pt-ammine complexes, and reaction of thiourea with 2 selected nucleobase complexes is reported. The relevance of these findings with respect to substitution reactions of Pt-nucleobase complexes and the nature of the tightly DNA-bound Pt, which cannot be removed by excess KCN, is discussed.

ACCESSION NUMBER: 1985:481346 CAPLUS
DOCUMENT NUMBER: 103:81346
TITLE: Reaction of cyanide with platinum-nucleobase complexes: preparative, spectroscopic, and structural studies. Unexpected stability of platinum-thymine and platinum-uracil complexes
AUTHOR(S): Raudaschl-Sieber, Gabriele; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganic Chemistry (1985), 24(15), 2426-32
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

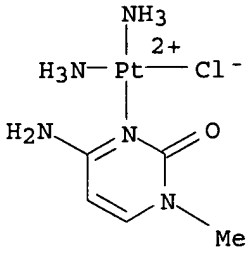
IT **96617-60-6P 96617-63-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 96617-60-6 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, (SP-4-3)-, (SP-4-1)-tetrakis(cyano-C)platinate(2-) (2:1) (9CI) (CA INDEX NAME)

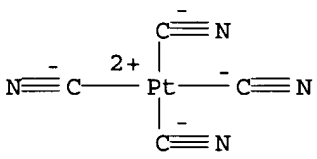
CM 1

CRN 75659-38-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

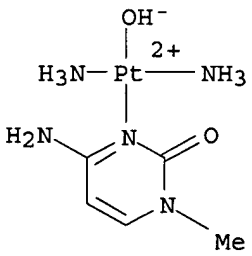
CRN 15004-88-3
CMF C4 N4 Pt
CCI CCS



RN 96617-63-9 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminehydroxy-, (SP-4-3)-, (SP-4-1)-tetrakis(cyano-C)platinate(2-) (2:1) (9CI) (CA INDEX NAME)

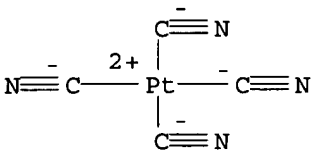
CM 1

CRN 80662-75-5
CMF C5 H14 N5 O2 Pt
CCI CCS

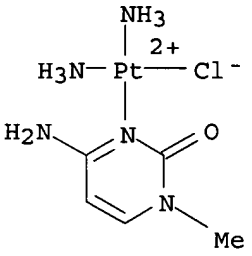


CM 2

CRN 15004-88-3
CMF C4 N4 Pt
CCI CCS

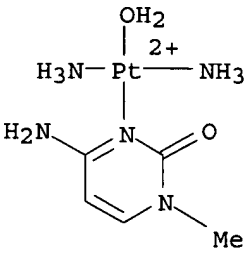


IT **75659-46-0 80662-70-0 80662-76-6**
85715-80-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanide, nucleobase release in relation to)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



● Cl⁻

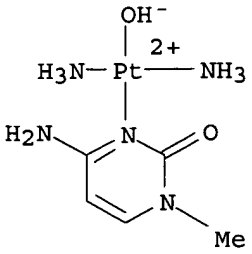
RN 80662-70-0 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 80662-76-6 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminehydroxy-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

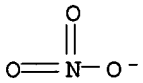
CM 1

CRN 80662-75-5
CMF C5 H14 N5 O2 Pt
CCI CCS



CM 2

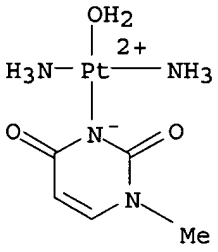
CRN 14797-55-8
CMF N O3



RN 85715-80-6 CAPLUS
CN Platinum(1+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

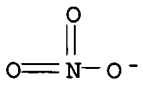
CM 1

CRN 85715-79-3
CMF C5 H13 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



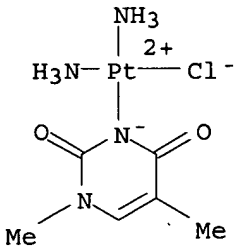
L7 ANSWER 69 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The title compd. is triclinic, space group P.hivin.1, with a 6.911(2), b 8.598(3), c 11.464(4) .ANG., .alpha. 100.13(3), .beta. 120.03(3), .gamma. 93.16(3).degree.; Z = 2. The structure was refined to R = 0.048 and Rw = 0.057. At. coordinates are given. The compd. contains the deprotonated 1-methylthymine ligand coordinated to Pt through N3 (1.973(10) .ANG.). This distance represents the shortest Pt-N3(pyrimidine-2,4-dione) bond reported so far. The 2 Pt-NH3 bond lengths differ significantly: Pt-NH3 (trans to Cl) is longer (2.052(10) .ANG. than Pg-NH3 (trans to N3 of 1-MeT)(2.002(11) .ANG.). The Pt-Cl distance (2.326(3) .ANG.) is normal, as is the large dihedral angle between the Pt coordination plane and the nucleobase (76.5.degree.).

ACCESSION NUMBER: 1985:446206 CAPLUS
DOCUMENT NUMBER: 103:46206
TITLE: X-ray structure of a mono(1-methylthyminato) complex of cisplatin, chloro(1-methylthyminato-N3)-cis-diammineplatinum(II) monohydrate
AUTHOR(S): Schoellhorn, Helmut; Thewalt, Ulf; Lippert, Bernhard
CORPORATE SOURCE: Sekt. Roentgen- Elektronenbeugung, Univ. Ulm, Ulm, D-79, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1985), 106(4), 177-80
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **97225-38-2**
RL: PRP (Properties)
(crystal structure of)

RN 97225-38-2 CAPLUS
CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-N3)-, monohydrate, (SP-4-3)- (9CI) (CA INDEX NAME)



• H_2O

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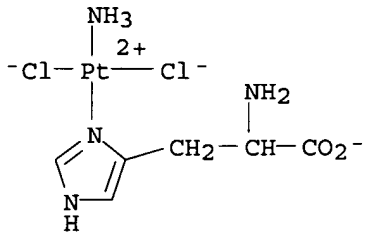
AB Various Pt(II)-L-histidine (HL) complexes were prepd. by reaction of K2PtCl4 (I) or cis-[Pt(NH3)2Cl2] (II) with HL and analyzed by 1H and 13C NMR spectroscopy, electrophoresis, and ion-exchange chromatog. HL may be coordinated to Pt by the imidazole imino group and/or the .alpha.-amino group; the carboxy group always remains free. I reacted with HL and HCl to give 2 isomers of cis-Pt(HL)2Cl2 in which HL is coordinated through the amino N or imino N atom. II reacts with HL to give a mixt. of compds. including cis-Pt(NH3)2HL (III) and 3 isomers of cis-[Pt(NH3)2(HL)2]Cl2, differing in the monodentate mode of coordination of HL. The reaction of III with HCl gave 2 isomers of Pt(NH3)(HL)Cl2 in which HL is ligated to Pt by an amino or imino group. The methods applied are suitable for analyzing reactions of HL with II under model conditions similar to physiol. conditions.

ACCESSION NUMBER: 1985:124545 CAPLUS
DOCUMENT NUMBER: 102:124545
TITLE: The reaction of platinum antitumor drugs with selected nucleophiles. II. Preparation and characterization of coordination compounds of platinum(II) and L-histidine
AUTHOR(S): Saudek, V.; Pivcova, H.; Noskova, D.; Drobnik, J.
CORPORATE SOURCE: Inst. Macromol. Chem., Czech. Acad. Sci., Prague, 162 06, Czech.
SOURCE: Journal of Inorganic Biochemistry (1985), 23(1), 55-72
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **95381-03-6P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from platinum histidine complex and hydrochloric acid)

RN 95381-03-6 CAPLUS

CN Platinate(1-), amminedichloro(L-histidinato-N3)-, hydrogen, monohydrochloride (9CI) (CA INDEX NAME)

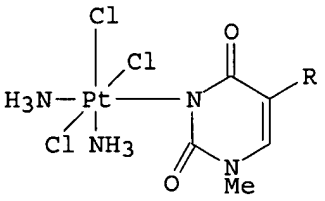


○ HCl

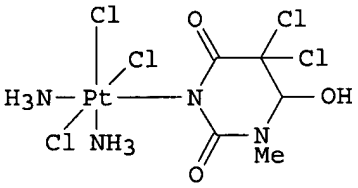
○ H+

ANSWER 71 OF 87 CAPLUS COPYRIGHT 2003 ACS

GI



II



III

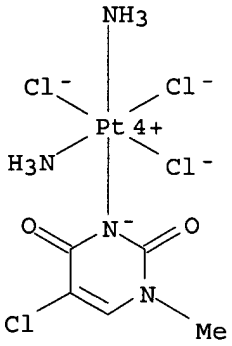
AB Reaction of cis-(NH3)2PtRCl (I; R = 1-methyluracil anion) with Cl2 in aq. soln. gave 3 Pt(IV)-uracil derivs. II (R = H, Cl) and III, depending on reaction conditions. In formation of II (R = H) from I and chlorine water, the expected oxidn. of Pt(II) to Pt(IV) took place. Treating of I with Cl gas gave II (R = Cl) in which the H at the C(5) position of the heterocyclic ring was replaced by Cl. In formation of III, from I and Cl in low yield, or from II (R = Cl) and Cl in good yield, HOCl added to the double bond of the uracil ligand. The x-ray crystal structures of II (R = Cl) and III, which were similar, showed exocyclic O atoms were locked between a pair of Cl ligands and one Cl and one NH3 ligand, resp., leading to small dihedral angles between the rings and the Pt(NH3)2ClN(3) plane.

ACCESSION NUMBER: 1985:24580 CAPLUS
DOCUMENT NUMBER: 102:24580
TITLE: cis-Diammineplatinum(IV) complexes of uracil through chlorine treatment of a platinum(II) complex: oxidative addition to the metal and modification (chlorine substitution, hypochlorous acid addition) of the nucleobase
AUTHOR(S): Mueller, Gerhard; Riede, Juergen; Beyerle-Pfnuer, Rut; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1984), 106(25), 7999-8001
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:24580

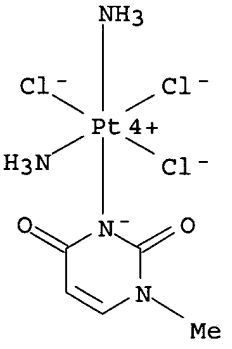
IT **93474-05-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

RN 93474-05-6 CAPLUS

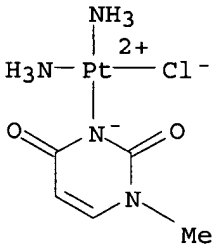
CN Platinum, diamminetrichloro(5-chloro-1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-31)- (9CI) (CA INDEX NAME)



IT **93474-04-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 93474-04-5 CAPLUS
CN Platinum, diamminetrichloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (OC-6-31)- (9CI) (CA INDEX NAME)



IT **85715-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorine, oxidative addn. and ligand chlorination in)
RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



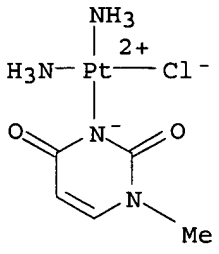
L7 ANSWER 72 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The mixed-nucleobase complex cis-[Pt(NH3)2LL1]NO3 (I; L = 1-methylcytosine-N3; HL1 = 1-methyluracil) was prepd. and characterized by 1H NMR, IR, and Raman spectroscopy. NMR spectra show that in acidic medium the 1-methyluracilate ligand becomes protonated (pKa .simeq. 0.9) and in a slow secondary reaction releases neutral 1-methyluracil. The pKa of the NH2 (N4) group of N3-platinated 1-methylcytosine in I was estd. to be .gtoreq.14. In the presence of Cu(II), I forms {[Pt(NH3)2L1]2(.mu.-L)Cu}(NO3)4.6H2O (II). II crystallizes in space group P.hivin.1, with a 11.522(6), b 10.924(4), c 10.736(2) .ANG., .alpha. 91.51(3), .beta. 109.08(3), .gamma. 114.43(3).degree., and Z = 1. The structure was refined to R = 0.051 and R.omega. = 0.054 on the basis of 2603 reflections. Both Pt atoms are bound to N3 of 1-methyluracil and N3 of 1-methylcytosine, resp., while Cu bonds to O4 of uracil and O2 of cytosine in pairs. All 3 metals have square-planar coordination spheres, with Cu sitting in the inversion center of the Pt2Cu unit. The Pt-Cu distances within the cation are 2.681(1) .ANG.. Cu-O distances to 1-methyluracil (1.931(12) .ANG.) and 1-methylcytosine (1.988(9) .ANG.) do not differ greatly. EPR spectra, at X- and Q-band frequencies, are consistent with a tetragonally elongated ligand field about the Cu2+ ion in II, and also in the related complexes cis-[(NH3)2Pt(HL1)2Cu(HL1)2Pt(NH3)2]2+. The spectra are compared with those of the dinuclear complex cis-[(NH3)2Pt(HL1)2Cu(H2O)2]2+ for which a significant dipolar coupling between the Cu2+ ions in a centrosym. related pair of cations in the unit cell is obsd.

ACCESSION NUMBER: 1984:502885 CAPLUS
DOCUMENT NUMBER: 101:102885
TITLE: Formation, crystal structure, and EPR spectroscopic properties of a heteronuclear (Pt2,Cu) mixed-nucleobase (1-methylcytosine, 1-methyluracil) complex: bis[(.mu.-1-methyluracilato-N3,O4)(.mu.-1-methylcytosine-N3,O2)-cis-diammineplatinum(II)]copper(II) tetranitrate-6-water
AUTHOR(S): Lippert, Bernhard; Thewalt, Ulf; Schoellhorn, Helmut; Goodgame, David M. L.; Rollins, Robert W.
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganic Chemistry (1984), 23(18), 2807-13
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-78-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silver nitrate and methylcytosine)

RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



L7 ANSWER 73 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The reaction of cis-[(NH3)2Pt(1-MeU)H2O]+ and cis-[(NH3)2Pt(1-MeU)]22+ (head-tail) (1-MeUH = 1-methyluracil) with AgNO3 in aq. soln. was studied by 1H NMR spectroscopy. cis-[Pt2(NH3)4(1-MeU)2Ag2](NO3)4.2H2O (I) and cis-[Pt(NH3)2(NO3)(1-MeU)Ag]NO3 (II) contg. Pt(II) and Ag(I) bound to 1-MeU were isolated and characterized. I crystallizes in the monoclinic space group C2/c with Z = 4 and a 13.810(2), b 16.279(2), c 11.871(2) .ANG., and .beta. 95.58(1).degree.. The structure was refined on 1797 reflections to R = 0.051 and Rw = 0.056. The 1-MeU ligands, arranged in head-tail fashion, bridge 2 cis-(NH3)2PtII through N(3) and O(4) and are bound to Ag through O(2). The 4 heavy atoms are lined up within the mol. cation, giving rise to intramol. distances of 2.892(1) .ANG. for Pt-Pt and 2.853(2) .ANG. for Pt-Ag. Adjacent cations are related by a C2 symmetry operation, leading to an intermol. Ag-Ag sepn. of 3.954(3) .ANG., with NO3- bridging neighboring Ag atoms. The Pt coordination spheres show some deviation from pure square-planar toward a distorted tetrahedral geometry. II contains Pt(II) bound to 1-MeU through N(3) and Ag(I) coordinated through O(4) and/or O(2). IR and Raman spectra are used to support this interpretation, and the usefulness of vibrational spectroscopy for the study of heteronuclear Ptx,Agy,Lz complexes is critically examd. 1H NMR spectroscopy was used to study the effect of Ag(I) on the equil. 2cis-[NH3)2Pt(1-MeU)D2O]+ .dblharw. [(NH3)2Pt(1-MeU)]22+ (head-tail). The results indicate a competition between Ag(I) and Pt(II) for O(4) of 1-MeU, very much as in the system Ag(I)/cis-[(NH3)2Pt(1-MeU)]22+ (head-head).

ACCESSION NUMBER: 1984:220520 CAPLUS
DOCUMENT NUMBER: 100:220520
TITLE: Tridentate 1-methyluracil in a tetranuclear Pt2,Ag2 complex. Crystal structure and solution behavior of bis(.mu.-1-methyluracilato)bis(cis-diammineplatinum(II))disilver tetranitrate-2-water (head-tail), cis-[(NH3)2Pt(C5H5N2O2)Ag]2(NO3)4.cntdot. 2H2O
AUTHOR(S): Thewalt, Ulf; Neugebauer, Dietmar; Lippert, Bernhard
CORPORATE SOURCE: Anorg. Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganic Chemistry (1984), 23(12), 1713-18
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

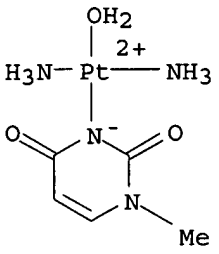
IT **85715-80-6**
RL: PRP (Properties)
(Raman spectra of)

RN 85715-80-6 CAPLUS

CN Platinum(1+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

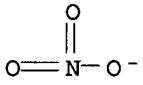
CM 1

CRN 85715-79-3
CMF C5 H13 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



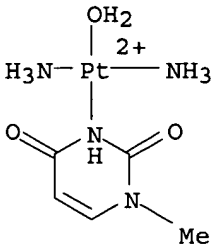
L7 ANSWER 74 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Time dependence studies, using high-performance liq. chromatog., on the reaction between cis-diamminediaquoplatinum [cis-Pt(NH3)2(H2O)22+] and guanine, N1-methylguanine, N7-methylguanine, N9-methylguanine, and N1,N7-dimethylguanine are reported. Each reaction gave rise to .gtoreq.8 compds.; the major components have been prepd., and characterization by 1H and 195Pt NMR has been attempted. Species of the form ((NH3)2Pt(NO3)-(G-H)-(NO3)-Pt(NH3)2+, (NH3)2Pt(G-H)(NO3) monomer, and (NH3)2Pt(G-H)(NO3) dimer, where G-H indicates the guanine monoanion, are postulated.

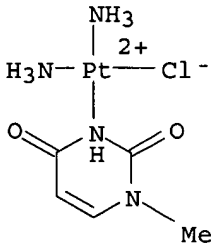
ACCESSION NUMBER: 1984:98471 CAPLUS
DOCUMENT NUMBER: 100:98471
TITLE: High-performance liquid chromatography studies on the interactions of cis-diamminediaquoplatinum ion (cis-Pt(NH3)2(H2O)22+) with guanine and methylated guanines
AUTHOR(S): Woollins, Ann; Rosenberg, Barnett
CORPORATE SOURCE: Dep. Biophys., Michigan State Univ., East Lansing, MI, USA
SOURCE: Journal of Inorganic Biochemistry (1984), 20(1), 23-37
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **89061-10-9 89061-11-0**
RL: PRP (Properties)
(NMR of)

RN 89061-10-9 CAPLUS
CN Platinum(2+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedione-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 89061-11-0 CAPLUS
CN Platinum(1+), diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedione-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



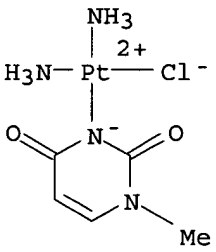
L7 ANSWER 75 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. of Pt(NH3)2(MeU)2 (I) [83350-97-4], [(NH3)2Pt(MeU)2Pt(NH3)2](NO3)2 (II) [75790-29-3], Pt(NH3)2Cl(MeU) (III) [**85715-78-2**] and (in soln.) [Pt(NH3)2(OH)(MeU)] (IV) [**87178-74-3**], (MeU = 1-methyluracil monoanion) is reported. Levels of 1-methyluracil [615-77-0] and I-IV in platinum-1-methyluracil blue (PtMeUB) were assessed by high performance liq. chromatog. (HPLC). This technique was used to show that in physiol. saline or water, PtMeUB hydrolyzes to III or IV, resp. Visible spectroscopy showed that the rate of hydrolysis of PtMeUB was much faster in fetal calf serum than in saline or water, with HPLC indicating that the product of hydrolysis in serum was III. The ppt. obtained upon treatment of DNA solns. with PtMeUB hydrolyzed to III or IV when suspended in saline or water. Compds. I-III were tested against the Ascites S-180J tumors, with II and III being active, while IV reacted readily with DNA. Possible mechanisms of the antitumor action of PtMeUB that involve III and IV are proposed.

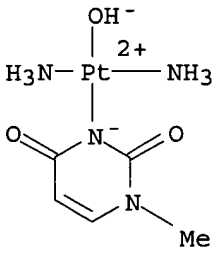
ACCESSION NUMBER: 1983:533352 CAPLUS
DOCUMENT NUMBER: 99:133352
TITLE: Interactions of platinum-1-methyluracil blue and its hydrolysis products with DNA
AUTHOR(S): Woollins, J. Derek; Rosenberg, Barnett
CORPORATE SOURCE: Dep. Biophys., Michigan State Univ., East Lansing, MI, USA
SOURCE: Journal of Inorganic Biochemistry (1983), 19(1), 41-9
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-78-2P 87178-74-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and antitumor activity of, DNA interaction in relation to)

RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 87178-74-3 CAPLUS
CN Platinum, diamminehydroxy(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)


OH -
2+
H3N— Pt — NH3
O
N -
O
N
Me

ANSWER 76 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. of several Pt(II) complexes of 1-methyluracil (HL) is reported: cis-Pt(NH3)2LCl.H2O (I) formed on addn. of 1 equiv of HCl to an aq. soln. of cis-Pt(NH3)2L2 on mild warming. Removal of the Cl- ligand from I with Ag+ gave, depending upon the reaction conditions, cis-[Pt(NH3)2(L)H2O]+, cis-[Pt(NH3)2L]22+ (head-tail) (II), and cis-[(NH3)2LPt(OH)PtL(NH3)2]+ (III). Addn. of cis-[Pt(NH3)2(H2O)2]2+ to cis-Pt(NH3)2L2 gave the head-head dimer cis-[Pt(NH3)2L]22+ (IV). The formation of dimers II-IV is pH-dependent: II and IV are favored under acidic pH conditions, whereas III is the major species at around neutral pH. 1H NMR, IR and in particular Raman spectroscopy were used to differentiate between mono- and bidentate binding of L in the various complexes. The crystal structure of the IV (NO3- salt, monohydrate) was detd. IV crystallizes in the space group P21/c with a 10.922(2), b 15.677(3), c 14.491(2) .ANG., .beta. 116.31(1).degree., Z = 4. The structure was refined on 2864 reflections to R = 0.082. Binding of L to the 2 Pt atoms occurs through N3 and O4. The non-coordinating O2 oxygens participate in H bond formation with the NH3 groups of the adjacent dimer.

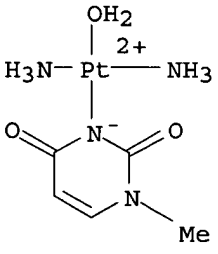
ACCESSION NUMBER: 1983:226882 CAPLUS
DOCUMENT NUMBER: 98:226882
TITLE: Formation of dinuclear (head-head,head-tail,.mu.-hydroxo) complexes of cis-diammineplatinum(II) with 1-methyluracil
AUTHOR(S): Lippert, Bernhard; Neugebauer, Dietmar; Raudaschl, Gabriele
CORPORATE SOURCE: Anorg. Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1983), 78(4), 161-70
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **85715-83-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dimerization of)

RN 85715-83-9 CAPLUS
CN Platinum(1+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

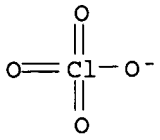
CRN 85715-79-3
CMF C5 H13 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-73-0

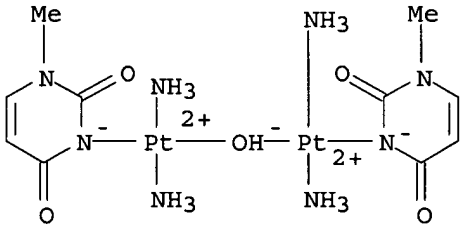
CMF Cl O4



IT **85715-82-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and Raman spectrum of)
RN 85715-82-8 CAPLUS
CN Platinum(1+), tetraammine-.mu.-hydroxybis(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)di-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

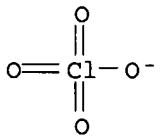
CM 1

CRN 85715-81-7
CMF C10 H23 N8 O5 Pt2
CCI CCS

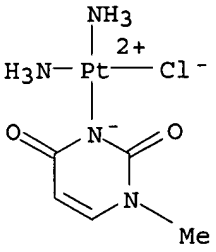


CM 2

CRN 14797-73-0
CMF Cl O4



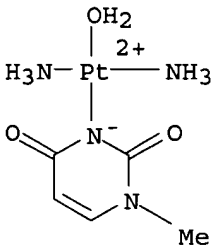
IT **85715-78-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with silver nitrate)
RN 85715-78-2 CAPLUS
CN Platinum, diamminechloro(1-methyl-2,4(1H,3H)-pyrimidinedionato-.kappa.N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **85715-80-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., Raman spectrum and isomerization and dimerization of)
RN 85715-80-6 CAPLUS
CN Platinum(1+), diammineaqua(1-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

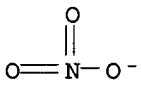
CM 1

CRN 85715-79-3
CMF C5 H13 N4 O3 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



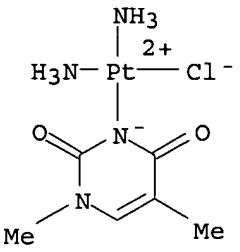
L7 ANSWER 77 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. is described of possible crosslinking products of cis-Pt(II) with the 1-methylthymine anion (T) as one base, and 1-methylcytosine (C), 9-ethylguanine (G), and 9-methyladenine (A), resp., as the second base. 1H NMR spectra are used to assign the donor atoms of the nucleobases in these complexes: T in all cases is bound to Pt through N3, C through N3, G through N7, and with A through N7 (monodentate), N1 (monodentate), and N7, N1 (bridging). Protonation of cis-[Pt(NH3)2T(A-(N7)]+ gives cis-[Pt(NH3)2T(HA-N7)]2+, a complex contg. a protonated A ligand. Warming of this complex leads to a H transfer from HA to T and subsequent elimination of neutral HT. This occurs both in H2O and Me2SO as solvents. With Me2SO, in a secondary reaction, NH3 is released from the complex and deprotonates the still available HA ligand eventually giving NH4+.

ACCESSION NUMBER: 1982:537603 CAPLUS
DOCUMENT NUMBER: 97:137603
TITLE: Mixed nucleobase complexes cis-Pt(NH3)2TX with T = 1-methylthymine anion and X = 1-methylcytosine, 9-ethylguanine, 9-methyladenine and 9-methyladeninium cation
AUTHOR(S): Beyerle, Rut; Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1982), 66(5), 141-6
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **77018-01-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with silver salts and nucleobases)

RN 77018-01-0 CAPLUS
CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



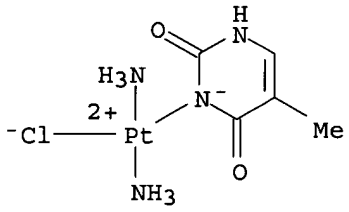
L7 ANSWER 78 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The complex-forming properties of the thyminate anion with cis- and trans-Pt(NH3)22+ in DMF and alk. aq. soln., and of (NH3)3Pt2+ in H2O, were studied using IR, Raman, UV, 1H NMR spectroscopy and HPLC (high-pressure liq. chromatog.). Complexes contg. thymine mono- and dianions bound to Pt via N1, via N3 and bridging through N3 + N1 were prepd., as well as 2 complexes contg. thymine monoanions as counter ions. The N1 and N3 binding of the thymine monoanion can be differentiated by 1H NMR and UV spectroscopy. Using HPLC, 3 different bis(thyminato) complexes of cis-Pt(NH3)22+ contg. the 2 tautomers of thymine monoanion (HT) were isolated and identified: cis-Pt(NH3)2(HT-N1)2, cis-Pt(NH3)2(HT-N1)(HT-N3), and cis-Pt(NH3)2(HT-N3)2. Binding of the HT tautomers is affected by the solvent used, by pH (with H2O being the solvent), the solubilities of the complexes formed, by the reaction time, and by H-bonding properties of adjacent ligands.

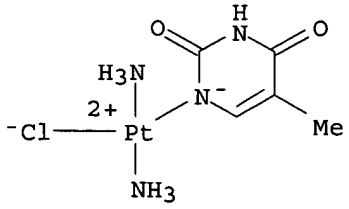
ACCESSION NUMBER: 1982:503244 CAPLUS
DOCUMENT NUMBER: 97:103244
TITLE: Platinum(II) complexes of thymine: factors influencing binding sites and methods of differentiation
AUTHOR(S): Pfab, Rudolf; Jandik, Peter; Lippert, Bernhard
CORPORATE SOURCE: Anorg. Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1982), 66(6), 193-204
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **82681-71-8P 82729-68-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reactions with 1-methylcytosine and ammonia)

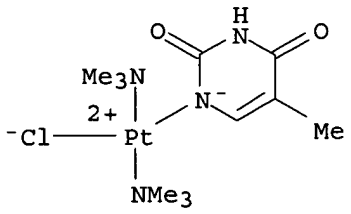
RN 82681-71-8 CAPLUS
CN Platinum, diamminechloro(5-methyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-2)- (9CI) (CA INDEX NAME)



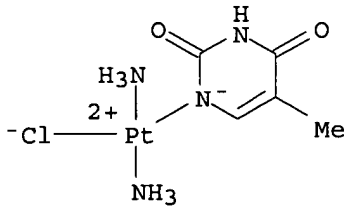
RN 82729-68-8 CAPLUS
CN Platinum, diamminechloro(5-methyl-2,4(1H,3H)-pyrimidinedionato-N1)-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **82848-54-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, by reaction of dichlorobis(trimethylamine)platinum with potassium thyminate)
RN 82848-54-2 CAPLUS
CN Platinum, chlorobis(N,N-dimethylmethanamine)(5-methyl-2,4(1H,3H)-pyrimidinedionato-N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT **72784-07-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aq. ammonia)
RN 72784-07-7 CAPLUS
CN Platinum, diamminechloro(5-methyl-2,4(1H,3H)-pyrimidinedionato-N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



ANSWER 79 OF 87 CAPLUS COPYRIGHT 2003 ACS

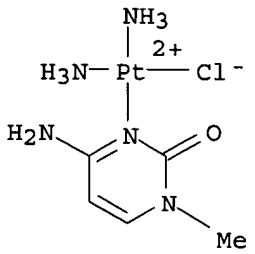
AB cis-[Pt(NH3)2L2]X2 (X = Cl- and NO3-, L = 1-methylcytosine-N3) were prepd., and the crystal structure of 1 of these was performed. cis-[Pt(NH3)2L2](NO3)2.L crystallizes in space group P.hivin.1, with a 14.020(3), b 13.676(3), c 7.031(3) .ANG., .alpha. 98.97(3).degree., .beta. 95.39(3).degree., .gamma. 110.16(2).degree., and Z = 2. The structure was detd. by std. methods and refined to R1 = 0.0488 and R2 = 0.0581 based on 5025 independent reflections. Data were collected by using Mo K.alpha. radiation and a Syntex P21 diffractometer. The structure shows 2 1-methylcytosine ligands coordinated to Pt through N(3) with normal Pt-N lengths of 2.032(8) and 2.045(6) .ANG. and in addn. a 1-methylcytosine mol. H bonded in the crystal lattice. The dihedral angles between the 2 bonded cytosine rings and between the rings and the ligand square plane are 102.0(3), 78.7(3), and 77.6(3).degree., resp. The presence of both coordinated and "free" ligand in the compd. permited a detailed study of the effects of N(3) platination on the 1-methylcytosine ring. Though the x-ray results do not show significant perturbations of the cytosine ring upon N(3) platination, 1H NMR, IR, and Raman spectroscopy do show distinct differences of the 2 species. Raman frequency shifts characteristic for N(3) platination both in soln. and in the solid state are reported and supported by comparison with the spectra of cis-[Pt(NH3)2L2]X2 (X = Cl-, NO3-), trans-[Pt(NH3)2L2](NO3)2, and cis-[PtCl(NH3)L]X (X = Cl-, NO3-).

ACCESSION NUMBER: 1982:465384 CAPLUS
DOCUMENT NUMBER: 97:65384
TITLE: Bis(1-methylcytosine) complexes of cis-diammineplatinum(II) and the x-ray structure of a platinum complex with covalently and hydrogen-bonded 1-methylcytosine, cis-diamminebis(1-methylcytosine-N3)platinum(II) dinitrate-1-methylcytosine, cis-[Pt(NH3)2(C5N7N3O)2](NO3)2.(C5H7N3O)
AUTHOR(S): Faggiani, R.; Lippert, B.; Lock, C. J. L.
CORPORATE SOURCE: Inst. Mater. Res., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Inorganic Chemistry (1982), 21(8), 3210-16
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **75659-46-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 75659-46-0 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



O Cl -

L7 ANSWER 80 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The prepn. of cis-diammine(1-methylcytosine-N3)platinum(II) complexes contg. terminal H2O, OH, and NO3 groups, resp., as 4th ligands, is reported: cis-[Pt(NH3)2L(H2O)](NO3)2.cntdot.H2O (I), cis-[Pt(NH3)2L(NO3)]NO3, cis-[Pt(NH3)2L(OH)]NO3.cntdot.2H2O (II), and cis-[Pt(NH3)2L(OH)]NO3 (L = 1-methylcytosine). The x-ray structures of I and II were detd. I crystallizes in the triclinic form: P.hivin.1, a 12.380(6), b 6.580(3), c 10.895(3) .ANG., .alpha. 90.39(3), .beta. 110.26(3), .gamma. 114.68(3).degree., Z = 2. II was obtained as monoclinic crystals, P21/c, a 12.207(4), b 6.203(1), c 18.853(5) .ANG., .beta. 109.64(2).degree.. Data for both crystals were collected with MoK.alpha. radiation. The crystal structures were detd. by std. methods; that of I was refined to R1 = 0.0575, R2 = 0.0610 based on 3442 independent reflections and that of II to R1 = 0.0657, R2 = 0.0688 based on 3100 independent reflections. The structures of the 2 cations are very similar with the pyrimidine plane at roughly right angles to the ligand square plane. Bond lengths (Pt-N, 2.02(1)-2.036(8) .ANG.; Pt-O 2.027(9), 2.052(8) .ANG.) are normal. I and II represent the 1st examples of Pt(II) complexes contg. terminal H2O and OH ligands, resp., that have been characterized with x-ray techniques. Their formation was made possible by the specific H-bonding properties of H2O and OH ligand in these complexes, and by poor donor strength of 02 of the 1-methylcycosine towards Pt in aq. soln. When warmed II is readily transferred into compds. contg. the N4-deprotonated L ligand as a bridge. Brief IR and Raman spectroscopic data are presented which enabled predictions on the structures of I and II before verification by x-ray anal.

ACCESSION NUMBER: 1982:173281 CAPLUS
DOCUMENT NUMBER: 96:173281
TITLE: Platinum(II) complexes with terminal hydroxo and aqua groups: crystal structures of hydroxo-cis-diammine(1-methylcytosine-N3)platinum(II) nitrate dihydrate, [Pt(OH)(NH3)2(C5H7N3O)]NO3.2H2O, and cis-diammineaqua(1-methylcytosine-N3)platinum(II) dinitrate hydrate, [Pt(NH3)2(H2O)(C5H7N3O)](NO3)2.H2O
AUTHOR(S): Britten, J. F.; Lippert, B.; Lock, C. J. L.; Pilon, P.
CORPORATE SOURCE: Inst. Mater. Res., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Inorganic Chemistry (1982), 21(5), 1936-41
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **80662-72-2P 80662-77-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

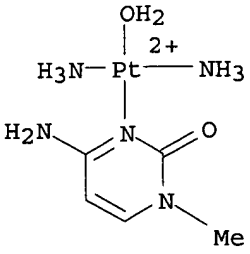
RN 80662-72-2 CAPLUS
CN Platinum(2+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diammineaqua-, (SP-4-3)-, dinitrate, monohydrate (9CI) (CA INDEX NAME)

CM 1

CRN 80662-71-1
CMF C5 H15 N5 O2 Pt . 2 N O3

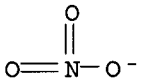
CM 2

CRN 80662-70-0
CMF C5 H15 N5 O2 Pt
CCI CCS



CM 3

CRN 14797-55-8
CMF N O3



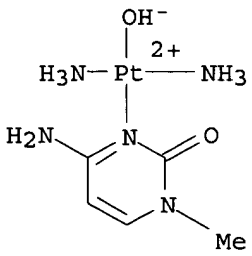
RN 80662-77-7 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminehydroxy-, (SP-4-3)-, nitrate, dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 80662-76-6
CMF C5 H14 N5 O2 Pt . N O3

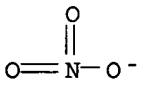
CM 2

CRN 80662-75-5
CMF C5 H14 N5 O2 Pt
CCI CCS



CM 3

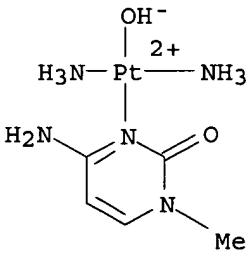
CRN 14797-55-8
CMF N O3



IT **80662-76-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 80662-76-6 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminehydroxy-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

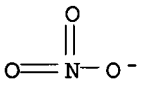
CM 1

CRN 80662-75-5
CMF C5 H14 N5 O2 Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



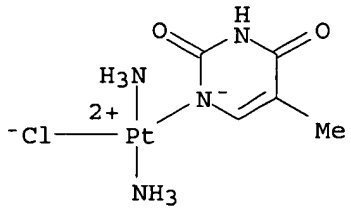
L7 ANSWER 81 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB High-performance liq. chromatog. (HPLC) studies on Pt thymine blues indicate that typical prepns. of this compd. contain several colorless Pt compds. (whites) and a no. of blue species. HPLC studies of the whites obtained from the reaction of cis-Pt(NH3)2Cl2 with thymine (HL) indicate the formation of cis-Pt(NH3)2L2 and cis-Pt(NH3)2ClL as well as cis-Pt(NH3)2(NO3)L formed during elution. The blues are ionic in nature and the compn. of the Pt thymine blue is concn., pH, and time dependent.

ACCESSION NUMBER: 1982:173254 CAPLUS
DOCUMENT NUMBER: 96:173254
TITLE: High-performance liquid chromatography studies on platinum thymine blue
AUTHOR(S): Woollins, J. Derek; Rosenberg, Barnett
CORPORATE SOURCE: Dep. Biophys., Michigan State Univ., East Lansing, MI, 48824, USA
SOURCE: Inorganic Chemistry (1982), 21(3), 1280-2
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **72784-07-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 72784-07-7 CAPLUS
CN Platinum, diamminechloro(5-methyl-2,4(1H,3H)-pyrimidinedionato-N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



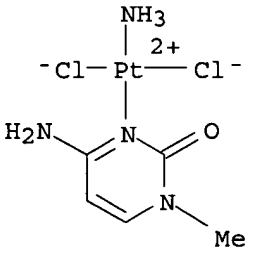
ANSWER 82 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB [Pt(NH3)C3](ClO4)2 (C = 1-methylcytosine) was prepd. by sequential treatment of trans-Pt(NH3)CCl2 with AgClO4 and C. Analogously obtained was trans-[Pt(NH3)CG2](ClO4)2 (G = 9-ethylguanine).

ACCESSION NUMBER: 1982:35500 CAPLUS
DOCUMENT NUMBER: 96:35500
TITLE: Tris(nucleobase) complexes derived from cis-diammineplatinum(II) chloride
AUTHOR(S): Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ., Garching, D-8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1981), 56(2), L23-L24
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **80103-36-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential reaction of, with silver perchlorate and 1-methylcytosine)

RN 80103-36-2 CAPLUS
CN Platinum, (4-amino-1-methyl-2(1H)-pyrimidinone-N3)amminedichloro-, (SP-4-1)- (9CI) (CA INDEX NAME)



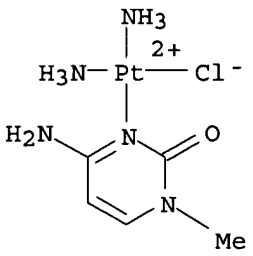
L7 ANSWER 83 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB The 1H NMR spectra of several cis-diammineplatinum(II) complexes of the model nucleobases 9-ethylguanine (G) and 1-methylcytosine (C) in Me2SO are reported: cis-[Pt(NH3)2G2](ClO4)2, cis-[Pt(NH3)2GC](ClO4)2, cis-[Pt(NH3)2(GH)C]ClO4, and cis-[{Pt(NH3)2GC}{Pt(NH3)2(GH)C}](ClO4)3. In all the complexes Pt is bound to G via N7 and to C via N3. Deprotonation of the G ligand at N1 is facilitated through Pt coordination at N7 (pK = 8.2, compared to 9.8 for the free G). The H-bonding behavior of the Pt complexes toward G, C, and 1-methylthymine (T) was studied in Me2SO by 1H NMR spectroscopy. Downfield shifts of the protons involved in H bonding were used as a qual. estn. of the stability of H bonding and compared with the Watson-Crick G-C base pair in the same solvent. The G ligand undergoes profound changes in its H-bonding pattern when coordinated to Pt though N7. H bonding with C is reduced and almost completely prevented when the G ligand is deprotonated at N1. There is also a complete loss of selectivity for G-C base pairing, as indicated by H bonding of the neutral G ligand with T and of the anionic G ligand with T and G. In particular, the novel H-bonding scheme between the platinated guanine anion and neutral guanine, which involves 3 H bonds, is quite strong. The cis-diammine groups contribute to the obsd. loss of G-C base pairing selectivity.

ACCESSION NUMBER: 1981:620027 CAPLUS
DOCUMENT NUMBER: 95:220027
TITLE: Effects of N7 platinum binding on the hydrogen-bonding behavior of 9-ethylguanine
AUTHOR(S): Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1981), 103(19), 5691-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **75659-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with sulfur perchlorate)

RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



⊖ Cl -

ANSWER 84 OF 87 CAPLUS COPYRIGHT 2003 ACS

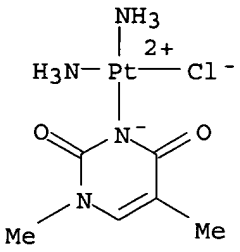
AB Bis(1-methylthyminato-N3)-cis-diammineplatinum(II), cis-Pt(NH3)2(C6H7N2O2)2, is readily protonated to give a compd. of compn. cis-[Pt(NH3)2(C6H7N2O2)(C6H8N2O2)]+X- (X = Cl-, NO3-, ClO4-). The compd. contains an anionic 1-methylthyminato ligand and a neutral 1-methylthymine ligand in an unusual iminol tautomer structure, both being coordinated to Pt(II) through N(3). The neutral thymine ligand is only weakly bound to Pt(II) and readily displaced. Spectroscopic data (1H NMR, UV, IR) are presented. A model for a possible nucleobase mispairing mechanism catalyzed through metal coordination at N(3) of thymidine is proposed.

ACCESSION NUMBER: 1981:166756 CAPLUS
DOCUMENT NUMBER: 94:166756
TITLE: Rare iminol tautomer of 1-methylthymine through metal coordination at N(3)
AUTHOR(S): Lippert, Bernhard
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1981), 55(1), 5-14
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **77018-01-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 77018-01-0 CAPLUS

CN Platinum, diamminechloro(1,5-dimethyl-2,4(1H,3H)-pyrimidinedionato-N3)-, (SP-4-3)- (9CI) (CA INDEX NAME)



L7 ANSWER 85 OF 87 CAPLUS COPYRIGHT 2003 ACS

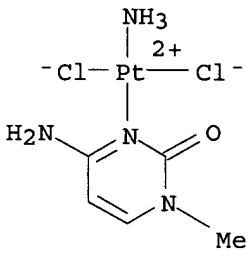
AB Two trans-ligand Pt(II) complexes were isolated and studied. trans-PtCl2(NH3)L.0.5H20 (I) (L = 1-methylcytosine-N3) has the space group C2/c with a 14.697(6), b 6.816(1), c 23.225(4) .ANG., .beta. 112.03(2).degree., and Z = 8. trans-[Pt(NH3)2L](NO3)2 (II) has space group P21/c with a 6.834(2), b 10.315(2), c 13.349(3) .ANG., .beta. 107.90(2).degree., and Z = 2. Data for both compds. were collected with use of Mo K.alpha. radiation and a Syntex P21 diffractometer. Both crystal structures were detd. by std. methods. I was refined to R1 = 0.0612 and R2 = 0.0775 on the basis of 2503 independent reflections. The final R1 = 0.0346 and R2 = 0.0410 for II were based on 1687 independent reflections. I has normal bond distances [Pt-Cl = 2.288(5), 2.296(5) .ANG.; Pt-N(pyrimidine) = 2.03(1) .ANG.; Pt-N(ammonia) = 2.04(1) .ANG.] and angles, and the pyrimidine ring is at an angle of 64.degree. to the ligand square plane. I is formed from cis-[Pt(NH3)2ClL]Cl in aq. soln. at room temp. A mechanism is proposed for its formation, and possible implications with regard to the binding properties of cis-Pt(NH3)2Cl2 are discussed. II also has normal bond distances [Pt-N(ammonia) = 2.067(10 .ANG.; Pt-N(pyrimidine) = 2.023(8) .ANG.] and angles; the pyrimidine-square-plane dihedral angle is larger (78.degree.).

ACCESSION NUMBER: 1981:149402 CAPLUS
DOCUMENT NUMBER: 94:149402
TITLE: Crystal structures of trans-dichloroammine(1-methylcytosine-N3)platinum(II) hemihydrate, [PtCl2(NH3)(C5H7N3)].1/2H2O, and trans-diamminebis(1-methylcytosine-N3)platinum(II) dinitrate. Evidence for the unexpected lability of ammonia in a cis-diammineplatinum(II) complex
AUTHOR(S): Lippert, B.; Lock, C. J. L.; Speranzini, R. A.
CORPORATE SOURCE: Inst. Mater. Res., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Inorganic Chemistry (1981), 20(3), 808-13
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **76068-65-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

RN 76068-65-0 CAPLUS

CN Platinum, (4-amino-1-methyl-2(1H)-pyrimidinone-N3)amminedichloro-, hydrate (2:1), (SP-4-1)- (9CI) (CA INDEX NAME)



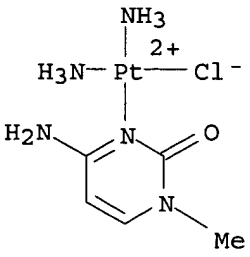
●1/2 H2O

IT **75659-46-0**
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with hydrochloric acid or sodium chloride and with 1-methylcytosine)

RN 75659-46-0 CAPLUS

CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)



E7 ANSWER 86 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Chloro-cis-diammine(1-methylcytosine-N3)platinum(II) nitrate, was prepd. in two monoclinic crystal forms: space group P21/c, with a 8.143(2), b 6.899(1), c 21.434(3) .ANG., .beta. 91.27(2).degree., Z = 4; and space group C2/c, with a 13.155(6), b 9.754(5), c 19.097(7) .ANG., .beta. 99.70(3).degree., Z = 8. The P21/c crystal was refined to R1 = 0.035, and R2 = 0.40 based on the basis of 3018 reflections and the C2/c crystal to to R1 = 0.47 and R2 = 0.064 on the basis of 1700 reflections. The cation, in both crystals, has a normal structure and bond lengths (Pt-N(ammonia) 2.04(1)-2.053(8), Pt-N(3) 2.026(6) 2.06(1), and Pt-Cl 2.299(2) 2.300(2) .ANG.). Both crystals contain a unit composed of two cations and two nitrate ions, both cations being H bonded to the same O atom of a nitrate group through a proton on 4-NH2 of the cytosine ring. Thus, both nitrate ions can be considered as bridging the two cations. The principal difference in the crystal packing is that in the P21/c structure this two cation-two anion unit is essentially planar, whereas in the C2/c structure it is bent about the nitrate-nitrate axis. 1H NMR spectra of the two compds. in D2O reveal a fast exchange of the C(5) proton of the 1-methylcytosine ligand with D ion upon heating. The corresponding C(5) deuterated 1-methylcytosine complexes were isolated and studied by IR spectroscopy.

ACCESSION NUMBER: 1981:75007 CAPLUS
DOCUMENT NUMBER: 94:75007
TITLE: Crystal structures of two crystalline forms of chloro-cis-diammine(1-methylcytosine-N3)platinum(II) nitrate, [PtCl(NH3)2(C5H7N3O)](NO3), and their proton NMR, IR, and Raman spectra
AUTHOR(S): Lippert, Bernhard; Lock, Colin James Lyne; Speranzini, Robert Anthony
CORPORATE SOURCE: Inst. Mater. Res., McMaster Univ., Hamilton, ON, L8S 4M1, Can.
SOURCE: Inorganic Chemistry (1981), 20(2), 335-42
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

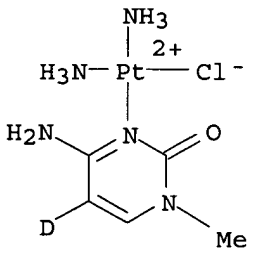
IT **75659-41-5 75659-43-7 75659-45-9**
RL: PRP (Properties)
(IR spectra of)

RN 75659-41-5 CAPLUS

CN Platinum(1+), [(4-amino-1-methyl-2(1H)-pyrimidinone-5-d)-N3]diamminechloro-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

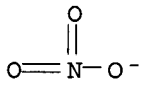
CM 1

CRN 75659-40-4
CMF C5 H12 Cl D N5 O Pt
CCI CCS



CM 2

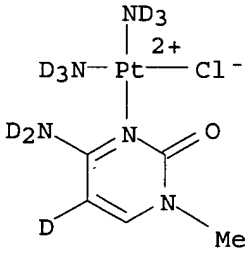
CRN 14797-55-8
CMF N O3



RN 75659-43-7 CAPLUS
CN Platinum(1+), [[4-(amino-d2)-1-methyl-2(1H)-pyrimidinone-5-d]-N3]di(ammine-d3)chloro-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

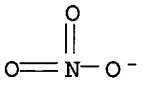
CM 1

CRN 75659-42-6
CMF C5 H4 Cl D9 N5 O Pt
CCI CCS



CM 2

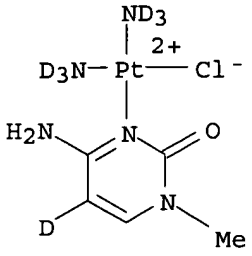
CRN 14797-55-8
CMF N O3



RN 75659-45-9 CAPLUS
CN Platinum(1+), [(4-amino-1-methyl-2(1H)-pyrimidinone-5-d)-N3]di(ammine-d3)chloro-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

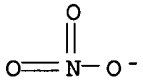
CM 1

CRN 75659-44-8
CMF C5 H6 Cl D7 N5 O Pt
CCI CCS

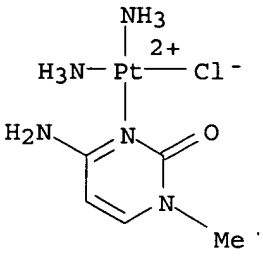


CM 2

CRN 14797-55-8
CMF N O3



IT **75659-46-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 75659-46-0 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, chloride, (SP-4-3)- (9CI) (CA INDEX NAME)

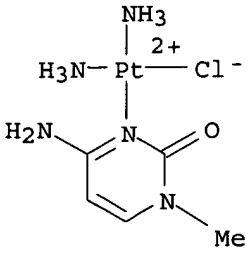


● Cl⁻

IT **75659-39-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., crystal structure and spectra of polymorphs of)
RN 75659-39-1 CAPLUS
CN Platinum(1+), (4-amino-1-methyl-2(1H)-pyrimidinone-N3)diamminechloro-, (SP-4-3)-, nitrate (9CI) (CA INDEX NAME)

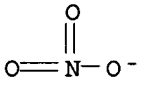
CM 1

CRN 75659-38-0
CMF C5 H13 Cl N5 O Pt
CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



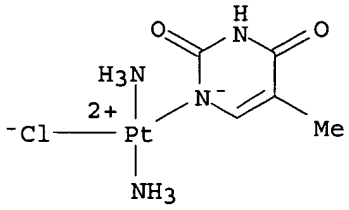
L7 ANSWER 87 OF 87 CAPLUS COPYRIGHT 2003 ACS

AB Pt(NH3)2LCl (I) (L = thymine) was prepd. by reaction of cis-Pt(NH3)2Cl2 with AgNO3 in DMF, filtration of AgCl, and addn. of KL. I was converted to cis-[Pt(NH3)2LL']ClO4 (II) (L' = 1-methylcytosine) which was characterized by chem. anal. and crystal structure detn. Pt is coordinated to thymine via the N(1) donor atom in both I and II. However, the antitumor platinum blues of unsubstituted 2,4-dihydroxypyrimidine contain ligands with N(1) donors as well as ligands with another donor (most likely N(3)) as the primary binding sites.

ACCESSION NUMBER: 1980:139918 CAPLUS
DOCUMENT NUMBER: 92:139918
TITLE: The role of N(1) coordinated thymine in 'platinum thymine blue'
AUTHOR(S): Lippert, Bernhard; Pfab, Rudolf; Neugebauer, Dietmar
CORPORATE SOURCE: Anorg.-Chem. Inst., Tech. Univ. Muenchen, Garching, 8046, Fed. Rep. Ger.
SOURCE: Inorganica Chimica Acta (1979), 37(1), L495-L497
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **72784-07-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(coordination sites and antitumor activity of)

RN 72784-07-7 CAPLUS
CN Platinum, diamminechloro(5-methyl-2,4(1H,3H)-pyrimidinedionato-N1)-, (SP-4-3)- (9CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                   395.47     791.58

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                                                       ENTRY    SESSION
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